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**ADVANCED SOFTWARE SUITE FOR
MULTIDISCIPLINARY
COMPUTATION**



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13. SUPPLEMENTARY NOTES THIS IS A SMALL BUSINESS INNOVATION RESEARCH (SBIR) PHASE I REPORT. This report contains color. The figures on page 27 are not available.					
14. ABSTRACT (Maximum 200 Words) The accomplishments of Phase I SBIR project on the development of a proposed high order multidisciplinary software suite are presented in this report. Several existing, but not necessarily high-order, upgradable target codes were first identified, with a synopsis of the numerical characteristics of the codes. The selection of the base code for the development of the proposed product was based on the type of numerical method (finite element/volume, finite difference), the initial capabilities of the codes, gird topology (structured/unstructured), and the structure of the code, vis-à-vis the incorporation of chimera/overset capabilities. The numerical kernels in the target codes were identified and a generalized flux function that supports the targeted applications was developed. A preliminary version of an elegant and intuitive graphics user interface (GUI) was also developed. To demonstrate feasibility of the proposed concept, a preliminary version of the multidisciplinary software suite was developed and tested for computational efficiency and accuracy against codes that are dedicated to magnetogasdynamics and aeroacoustics.					
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I. Introduction

The Thaerocomp Technical Corporation (TTC) has proposed to develop next-generation software that will revolutionize practical CFD-based analyses by providing the capability for seamless multidisciplinary simulation using highly accurate procedures. The software identifies, integrates, and then systematically upgrades common elements of major research codes, to yield a versatile high-order (Lele, 1991) software suite that can be used to simulate, in a coupled fashion, various elements of turbulence, electromagnetics, aeroacoustics, magnetogasdynamics, fluid-structure interaction, and chemically reacting flows. An elegant and intuitive graphical user interface (GUI) will be developed by leveraging experience derived from our flagship product INSTED. TTC's new, tightly integrated and versatile product will reduce the simulation time by orders of magnitude and drastically reduce the design cost of modern engineering systems requiring multidisciplinary optimization. The proposed software will facilitate out-of-the-box approaches by providing a validated realistic virtual environment, thus impacting all major thrusts of the Air Vehicles Directorate, including access-to-space, sustainment, and unmanned air vehicles.

The present document summarizes the accomplishments of the Phase I effort, which successfully and firmly established the feasibility of the concept proposed by TTC. In specifics, the following tasks were successfully carried out in Phase I:

- Identification of several existing, but not necessarily high order, upgradable target codes, with a synopsis of the numerical characteristics of the codes. For each code, several phone and written contacts were made in order to obtain the current status of the code.
- Selection of the base code for the development of the high order multidisciplinary software. The specific criteria for selection include a) the type of numerical method (finite element/volume, finite difference, spectral methods), b) capabilities of the codes, c) grid topology (structured/unstructured), d) the structure of the code, vis-à-vis the incorporation of

chimera/overset capabilities for competitive modeling of complex geometry and relative motion, e) the availability of the code.

- Identification of the numerical kernels in the codes and development of a generalized flux function that supports all the applications.
- Implementation of an elegant and intuitive graphics user interface (GUI) to demonstrate the feasibility of a user-friendly interface for the high order multidisciplinary software, which is an absolute necessity for commercialization of the final product.
- Development and testing of a preliminary version of the proposed software. A demonstration for MGD and Aeroacoustics is presented in terms of the computational efficiency and accuracy of computation when compared with codes that are dedicated to these applications.
- Investigation of marketing efforts for the commercial sector during Phase I, which shows that considerable interest exists for the proposed product because of its potential to ensure fast time-to-market.

II: Identification of Target Codes

The target codes for upgrade have been identified, as were the kernels in these codes. Some of these codes are listed in the table below, together with a synopsis of their numerical characteristics. Several contacts were made to find out the current state of the various codes. Dr. Pieter Buning (NASA Langley) provided an overview, current status, and the relationship between ARC3D code (originally developed by Tom Pulliam), XAIR (derivative of ARC3D), OVERFLOW (also a derivative of ARC3D), CFL3D (developed from NASA Langley), and WIND (originally developed by Douglas Ray Cosner/McDonnell Douglas). Greg Power (Contractor at AEDC) provided detailed information to TTC on the current status of WIND, which is the main production flow solver for the NPARC Alliance.

	ARC3D	FDL3DI	XAIR	OVERFLOW	WIND (NPARC)
	(NASA)	(WPAFB)	(AEDC)	(NASA)	(Boeing)
Method	FD	FD	FD	FD	FD (Node-based FV)
Spatial Scheme	Upwind, centered	Compact, centered, upwind	Upwind, centered	Upwind, centered	Upwind, centered,
Spatial accuracy	2 nd , probably 3 rd (Roe)	2 nd , 4 th , 6 th , etc.	2 nd , probably 3 rd (Roe)	2 nd , probably 3 rd (Roe)	2 nd , probably 3 rd (Roe)
Temporal scheme	Beam-Warming	Beam-Warming, RK4	Partial factorization + Gauss-Seidel	Beam-Warming	Partial factorization + point Jacobi or Gauss-Seidel
Time Accuracy	Steady state, second order with sub-iterations	RK4, 2 nd , 3 rd , time – accurate	2 nd , time-accurate moving grids	Steady state, 2 nd –order with sub-iterations	First-order, essentially
Stabilization	Explicit 4 th /2 nd dissipation, Inherent Roe	Compact filters, explicit 4/2	HLLE (Roe-like) upwinding	Explicit 4 th /2 nd dissipation, inherent Roe	Upwinding
Multiblock	No	Yes	Yes	Yes	Yes
Chimera, Overset Capabilities	None	Limited	Extensive	Extensive	Extensive

Turbulence modeling	RANS	LES	RANS	RANS	RANS
Matrix method	Scalarized pentadiagonal	TDMA	N/A	Scalarized pentadiagonal	N/A
Mesh interpolation tools	Limited	Limited	Extensive	Extensive	Extensive
Extent of dissipation	Significant	Slight	Significant	Significant	Significant
Applications	Standard Navier-Stokes, research, mostly in-house	Acoustics, DNS/LES, CEM, MHD, mostly in-house	In-house only, not supported	Extensive industry use	Part of NPARC, extensive industry use

On the basis of the numerical characteristics of the reviewed code, vis-à-vis the goal of this project, we selected the FDL3D code (Gaitonde and Visbal, 1998) as the basis for the development of the multidisciplinary CFD tool. The specific criteria used include the type of numerical method, the capabilities of the target code, grid topology in the code, chimera/overset capability and the availability of the code. Note that none of the versions of the FDL3D code is capable of multidisciplinary simulation. They also do not currently provide high-order shock-capturing capabilities. Furthermore, the overset/chimera capability is not as advanced as that in some of the other codes that we reviewed, notably OVERFLOW and WIND. The types of boundary conditions currently supported in FDL3D are limited, for example, when compared with WIND. These 4 areas were automatically added to the technical focus for the SBIR project. The WENO scheme (Shu, 1997) was selected for high order shock capturing.

III: Governing Equations and mathematical model

The Phase I proposal promised to develop a preliminary generalized framework for the multidisciplinary software, including a generalized flux function, and to select the platform for the high order calculations and for stabilization in flow fields with shocks and/or strong discontinuity. It was also planned to test a preliminary version of the software suite.

A preliminary version of the proposed module that supports generalized flux functions and source terms was developed in Phase I. The module uses the same high order procedure for evaluating the derivatives for the various flux functions (source terms). The analysis of the efficiency and accuracy of the generalized flux procedure relative that of the individual single applications was also started in Phase I. Each of the supported applications, in curvilinear coordinates, can be written in the form

$$\frac{\partial X'}{\partial \tau} + \frac{\partial F'}{\partial \xi} + \frac{\partial G'}{\partial \eta} + \frac{\partial H'}{\partial \zeta} = \frac{\partial F'_v}{\partial \xi} + \frac{\partial G'_v}{\partial \eta} + \frac{\partial H'_v}{\partial \zeta} + S',$$

where τ is the time domain, (ξ, η, ζ) are the transformed coordinates that respectively correspond to the physical coordinates (x, y, z) . F' , G' , and H' are the inviscid fluxes, while F'_v , G'_v , and H'_v are the fluxes associated with the stresses for a particular application. S' is a generic source term. Some manipulations are sometimes required in order convert the stresses into the foregoing form, notable examples being the *Maxwell's stresses* in MGD. The various flux functions that need to be “combined” are listed below, using F' as an example. The generalized flux functions for some of the multidisciplinary applications are presented subsequently.

DNS, non-MHD: When a handle to the module indicates *direct numerical simulation*, or the fluid component of a *fluid-structure interaction*, the module assumes the following definitions

$$X' = \frac{1}{J} \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix}, \quad F' = \begin{pmatrix} \rho U \\ \rho u U + \xi_x p \\ \rho v U + \xi_y p \\ \rho w U + \xi_z p \\ \rho(E + p)U - \xi_t p \end{pmatrix},$$

where

$$U = \xi_t + \xi_x u + \xi_y v + \xi_z w$$

LES, non-MHD: For non-MHD, LES problems, the following definitions apply (Germano et al., 1991; Rizetta et al, 2000, 2001):

$$X' = \frac{1}{J} \begin{bmatrix} \bar{\rho} \\ \bar{\rho} \tilde{u} \\ \bar{\rho} \tilde{v} \\ \bar{\rho} \tilde{w} \\ \bar{\rho} \tilde{E} \end{bmatrix}, \quad F' = \begin{pmatrix} \bar{\rho} \tilde{U} \\ \bar{\rho} \tilde{u} \tilde{U} + \xi_x \bar{p} \\ \bar{\rho} \tilde{v} \tilde{U} + \xi_y \bar{p} \\ \bar{\rho} \tilde{w} \tilde{U} + \xi_z \bar{p} \\ \bar{\rho} \tilde{E} \tilde{U} + \xi_x u_i \bar{p} \end{pmatrix}$$

where

$$\tilde{U} = \xi_t + \xi_x \tilde{u} + \xi_y \tilde{v} + \xi_z \tilde{w}$$

MGD: For a simplified MGD model, i. e., assuming chemical and thermal equilibrium, the appropriate definitions are (Gaitonde, 1999):

$$X' = \frac{1}{J} \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \\ B_x \\ B_y \\ B_z \end{bmatrix}, \quad F' = \frac{1}{J} \begin{pmatrix} \rho U \\ \rho u U + \xi_x p - \xi_x R_b \frac{B_x^2}{\mu_m} - \xi_y R_b B_x \frac{B_y}{\mu_m} - \xi_z R_b B_x \frac{B_z}{\mu_m} \\ \rho v U + \xi_y p - \xi_x R_b B_x \frac{B_y}{\mu_m} - \xi_y R_b \frac{B_y^2}{\mu_m} - \xi_z R_b B_y \frac{B_z}{\mu_m} \\ \rho w U + \xi_z p - \xi_x R_b B_x \frac{B_z}{\mu_m} - \xi_y R_b B_y \frac{B_z}{\mu_m} - \xi_z R_b \frac{B_z^2}{\mu_m} \\ (\rho E + p)U - \xi_x R_b (U \cdot \frac{\mathbf{B}}{\mu_m}) B_x - \xi_y R_b (U \cdot \frac{\mathbf{B}}{\mu_m}) B_y - \xi_z R_b (U \cdot \frac{\mathbf{B}}{\mu_m}) B_z \\ \xi_y (v B_x - u B_y) + \xi_z (w B_x - u B_z) \\ \xi_x (u B_y - v B_x) + \xi_z (w B_y - v B_z) \\ \xi_x (u B_z - w B_x) + \xi_y (v B_z - w B_y) \end{pmatrix}$$

The standard notations apply (see reference).

Species conservation: When reacting or non-reacting species have to be simulated, the module must branch to the following definitions:

$$X' = \frac{1}{J} \begin{bmatrix} \rho \phi_1 \\ \rho \phi_2 \\ \dots \\ \rho \phi_n \end{bmatrix}, \quad F' = \begin{pmatrix} \rho \phi_1 U \\ \rho \phi_2 U \\ \dots \\ \rho \phi_n U \end{pmatrix}$$

where, as before, we can define

$$U = \xi_t + \xi_x u + \xi_y v + \xi_z w.$$

Note that the species fluxes could easily be appended to any of the foregoing definitions, in a coupled approach, as opposed to the *segregated* manner implied here.

CEM: For the time-dependent electromagnetics, the modules sends controls to the Maxwell's equations for the electromagnetic field in free-space, which can be written as (Shang and Gaitonde, 1995, Gaitonde and Shang, 1997):

$$X' = \frac{1}{J} \begin{bmatrix} 0 \\ 0 \\ 0 \\ J_x \\ J_y \\ J_z \end{bmatrix}, \quad F' = \begin{pmatrix} \xi_y D_z / \epsilon - \xi_z D_y / \epsilon \\ -\xi_x D_z / \epsilon + \xi_z D_x / \epsilon \\ \xi_x D_y / \epsilon - \xi_y D_x / \epsilon \\ -\xi_y B_z / \mu_m + \xi_z B_y / \mu_m \\ \xi_x B_z / \mu_m - \xi_z B_x / \mu_m \\ -\xi_x B_y / \mu_m + \xi_y B_x / \mu_m \end{pmatrix}.$$

In these expressions, $\mathbf{B} = (B_x, B_y, B_z)$ is the vector of magnetic field density, $\mathbf{D} = (D_x, D_y, D_z)$ is the vector of electric displacement, μ_m is magnetic permeability, and ϵ is the electric permittivity.

The starting point for the completion of the generalized flux function in Phase II is the assembled functions, which are defined below:

$$\frac{\partial X'}{\partial \tau} + \frac{\partial F'}{\partial \xi} + \frac{\partial G'}{\partial \eta} + \frac{\partial H'}{\partial \zeta} = (1 - \pi_6 - \pi_7) \left[\frac{\partial F'_v}{\partial \xi} + \frac{\partial G'_v}{\partial \eta} + \frac{\partial H'_v}{\partial \zeta} \right] \\ + \pi_2 S_2 + \pi_3 S_3 + \pi_6 S_6 \equiv S,$$

	DNS	LES	CRF	MHD	CEM	CAA	FSI
$\pi_{1,j}$	1	0	0	0	0	0	0
$\pi_{2,j}$	0	1	0	0	0	0	0
$\pi_{3,j}$	0	0	1	0	0	0	0
$\pi_{4,j}$	0	0	0	1	0	0	0
$\pi_{5,j}$	0	0	0	1	0	0	0
$\pi_{6,j}$	0	0	0	0	1	0	0
$\pi_{7,j}$	0	0	0	0	0	1	0
$\pi_{8,j}$	0	0	0	0	0	0	1

In this table, the subscript “j” on π has been introduced to identify the columns. The abbreviations in the table are as follows:

Symbol	Description	Remarks
DNS	Direct numerical simulation	Standard Navier-Stokes Eqns
LES	Large eddy simulation	Standard Navier-Stokes Eqns
CRF	Chemically-reacting flow	Continuum
MGD	Magnetogasdynamics	Continuum
CEM	Computational electromagnetics	

CAA	Computational aeroacoustics	
FSI	Fluid-structure interaction	Structure equations will be included in the Phase II project

The complete flux functions for each of the applications are subsets of the following generalized functions derived during Phase I:

$$X' = \frac{1}{J} \begin{bmatrix} (\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5 + \pi_7)\rho + \pi_6 B_x \\ (\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5 + \pi_7)\rho u + \pi_6 B_y \\ (\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5 + \pi_7)\rho v + \pi_6 B_z \\ (\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5 + \pi_7)\rho w + \pi_6 J_x \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)\rho + (\pi_4 + \pi_5)\rho E_B + \pi_6 J_y \\ \pi_3 \rho Y_i + \pi_6 D_x + \pi_6 J_z \\ (\pi_4 + \pi_5)B_x \\ (\pi_4 + \pi_5)B_y \\ (\pi_4 + \pi_5)B_z \end{bmatrix}$$

The inviscid fluxes are

$$F' = \frac{1}{J} \begin{pmatrix} (\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5 + \pi_7)\rho U + \pi_6(\xi_y D_x/\epsilon - \xi_z D_y/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho u U + \xi_z p] + (\pi_4 + \pi_5)[\xi_x E_b - R_b \tilde{B}_x \frac{B_x}{\mu_m}] \\ + \pi_6(-\xi_x D_x/\epsilon + \xi_z D_z/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho v U + \xi_y p] + (\pi_4 + \pi_5)[\xi_y E_b - R_b \tilde{B}_y \frac{B_y}{\mu_m}] \\ + \pi_6(\xi_x D_y/\epsilon - \xi_y D_x/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho w U + \xi_z p] + (\pi_4 + \pi_5)[\xi_z E_b - R_b \tilde{B}_z \frac{B_z}{\mu_m}] \\ + \pi_6(-\xi_y B_x/\mu_m + \xi_z B_y/\mu_m) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)(\rho E + p)U + (\pi_4 + \pi_5)[2E_b U - R_b(\mathbf{U} \cdot \mathbf{B})\frac{\tilde{B}_x}{\mu_m}] \\ + \pi_6(\xi_x B_x/\mu_m - \xi_z B_z/\mu_m) \\ \pi_3[\rho Y_i U] + \pi_6(-\xi_x B_y/\mu_m + \xi_y B_z/\mu_m) \\ (\pi_4 + \pi_5)[v\xi_y + w\xi_z]B_x - u(\xi_y B_y + \xi_z B_z) \\ (\pi_4 + \pi_5)[(u\xi_x + w\xi_z)B_y - v(\xi_x B_x + \xi_z B_z)] \\ (\pi_4 + \pi_5)[(u\xi_x + v\xi_y)B_z - w(\xi_x B_x + \xi_y B_y)] \end{pmatrix}$$

$$G' = \frac{1}{J} \begin{pmatrix} (\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5 + \pi_7)\rho V + \pi_6(\eta_y D_x/\epsilon - \eta_z D_y/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho u V + \eta_z p] + (\pi_4 + \pi_5)[\eta_x E_b - R_b \tilde{B}_x \frac{B_x}{\mu_m}] \\ + \pi_6(-\eta_x D_x/\epsilon + \eta_z D_z/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho v V + \eta_y p] + (\pi_4 + \pi_5)[\eta_y E_b - R_b \tilde{B}_y \frac{B_y}{\mu_m}] \\ + \pi_6(\eta_x D_y/\epsilon - \eta_y D_x/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho w V + \eta_z p] + (\pi_4 + \pi_5)[\eta_z E_b - R_b \tilde{B}_z \frac{B_z}{\mu_m}] \\ + \pi_6(-\eta_y B_x/\mu_m + \eta_z B_y/\mu_m) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)(\rho E + p)V + (\pi_4 + \pi_5)[2E_b V - R_b(\mathbf{U} \cdot \mathbf{B})\frac{\tilde{B}_y}{\mu_m}] \\ + \pi_6(\eta_x B_x/\mu_m - \eta_z B_z/\mu_m) \\ \pi_3[\rho Y_i V] + \pi_6(-\eta_x B_y/\mu_m + \eta_y B_z/\mu_m) \\ (\pi_4 + \pi_5)[v\eta_y + w\eta_z]B_x - u(\eta_y B_y + \eta_z B_z) \\ (\pi_4 + \pi_5)[(u\eta_x + w\eta_z)B_y - v(\eta_x B_x + \eta_z B_z)] \\ (\pi_4 + \pi_5)[(u\eta_x + v\eta_y)B_z - w(\eta_x B_x + \eta_y B_y)] \end{pmatrix}$$

and

$$H' = \frac{1}{J} \begin{pmatrix} (\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5 + \pi_7)\rho W + \pi_6(\zeta_y D_z/\epsilon - \zeta_x D_y/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho u W + \zeta_x p] + (\pi_4 + \pi_5)[\zeta_x E_b - R_b \hat{B}_z \frac{E_x}{\mu_m}] \\ + \pi_6(-\zeta_x D_z/\epsilon + \zeta_x D_x/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho v W + \zeta_y p] + (\pi_4 + \pi_5)[\zeta_y E_b - R_b \hat{B}_z \frac{E_y}{\mu_m}] \\ + \pi_6(\zeta_x D_y/\epsilon - \zeta_y D_x/\epsilon) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)[\rho w W + \zeta_z p] + (\pi_4 + \pi_5)[\zeta_z E_b - R_b \hat{B}_z \frac{E_z}{\mu_m}] \\ + \pi_6(-\zeta_y B_z/\mu_m + \zeta_x B_y/\mu_m) \\ (\pi_1 + \pi_2 + \pi_3 + \pi_7)(\rho E + p)W + (\pi_4 + \pi_5)[2E_b W - R_b(\mathbf{U} \cdot \mathbf{B}) \frac{\hat{B}_z}{\mu_m}] \\ + \pi_6(\zeta_x B_z/\mu_m - \zeta_x B_x/\mu_m) \\ \pi_8[\rho Y_i W] + \pi_6(-\zeta_x B_y/\mu_m + \zeta_y B_x/\mu_m) \\ (\pi_4 + \pi_5)[v \zeta_y + w \zeta_x] B_z - u(\zeta_y B_y + \zeta_x B_x) \\ (\pi_4 + \pi_5)[(u \zeta_x + w \zeta_y) B_y - v(\zeta_x B_x + \zeta_y B_z)] \\ (\pi_4 + \pi_5)[(u \zeta_x + v \zeta_y) B_z - w(\zeta_x B_x + \zeta_y B_y)] \end{pmatrix}$$

The dissipative fluxes are as follows:

$$F'_v = \frac{1}{J} \begin{pmatrix} 0 \\ \frac{1}{R_e} \zeta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i1} + (\pi_2 + \pi_3) \sigma_{i1}^{LES}] \\ \frac{1}{R_e} \zeta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i2} + (\pi_2 + \pi_3) \sigma_{i2}^{LES}] \\ \frac{1}{R_e} \zeta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i3} + (\pi_2 + \pi_3) \sigma_{i3}^{LES}] \\ \frac{1}{R_e} (\zeta_{\alpha i} u_j [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{ij} + (\pi_2 + \pi_3) \sigma_{ij}^{LES}] \\ + (\gamma-1) \frac{1}{Pr} M^2 \frac{1}{R_e} \zeta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) q_i + (\pi_2 + \pi_3) Q_i^{LES}] \\ + (\pi_4 + \pi_5) \frac{R_g}{\mu_m R_i \sigma} \left[\zeta_{\alpha i} \frac{\partial}{\partial \alpha_i} \left(\frac{1}{2} \frac{B^2}{\mu_m} \right) - \zeta_{\alpha i} \left(\frac{\partial B_x}{\partial x \mu_m} + \frac{\partial B_y}{\partial y \mu_m} + \frac{\partial B_z}{\partial z \mu_m} \right) \right] \\ \frac{1}{R_e} \zeta_{\alpha i} [\pi_8 (\Phi_{ij} + \chi_{ij}^{LES})] \\ (\pi_4 + \pi_5) \frac{1}{R_e \sigma} \left[\zeta_y \frac{\partial B_x}{\partial y \mu_m} + \zeta_x \frac{\partial B_z}{\partial x \mu_m} - \zeta_y \frac{\partial B_z}{\partial x \mu_m} - \zeta_x \frac{\partial B_x}{\partial y \mu_m} \right] \\ (\pi_4 + \pi_5) \frac{1}{R_e \sigma} \left[\zeta_x \frac{\partial B_y}{\partial x \mu_m} + \zeta_z \frac{\partial B_z}{\partial z \mu_m} - \zeta_x \frac{\partial B_z}{\partial y \mu_m} - \zeta_z \frac{\partial B_y}{\partial x \mu_m} \right] \\ (\pi_4 + \pi_5) \frac{1}{R_e \sigma} \left[\zeta_x \frac{\partial B_z}{\partial x \mu_m} + \zeta_y \frac{\partial B_x}{\partial y \mu_m} - \zeta_x \frac{\partial B_x}{\partial z \mu_m} - \zeta_y \frac{\partial B_z}{\partial x \mu_m} \right] \end{pmatrix},$$

$$G'_v = \frac{1}{J} \begin{pmatrix} 0 \\ \frac{1}{R_e} \eta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i1} + (\pi_2 + \pi_3) \sigma_{i1}^{LES}] \\ \frac{1}{R_e} \eta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i2} + (\pi_2 + \pi_3) \sigma_{i2}^{LES}] \\ \frac{1}{R_e} \eta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i3} + (\pi_2 + \pi_3) \sigma_{i3}^{LES}] \\ \frac{1}{R_e} \eta_{\alpha i} u_j [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{ij} + (\pi_2 + \pi_3) \sigma_{ij}^{LES}] \\ + (\gamma-1) \frac{1}{Pr} M^2 \frac{1}{R_e} \eta_{\alpha i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) q_i + (\pi_2 + \pi_3) Q_i^{LES}] \\ + (\pi_4 + \pi_5) \frac{R_g}{\mu_m R_i \sigma} \left[\eta_{\alpha i} \frac{\partial}{\partial \alpha_i} \left(\frac{1}{2} \frac{B^2}{\mu_m} \right) - \eta_{\alpha i} \left(\frac{\partial B_x}{\partial x \mu_m} + \frac{\partial B_y}{\partial y \mu_m} + \frac{\partial B_z}{\partial z \mu_m} \right) \right] \\ \pi_8 \frac{1}{R_e} \eta_{\alpha i} [(\Phi_{ij} + \chi_{ij}^{LES})] \\ (\pi_4 + \pi_5) \frac{1}{R_e \sigma} \left[\eta_y \frac{\partial B_x}{\partial y \mu_m} + \eta_x \frac{\partial B_z}{\partial x \mu_m} - \eta_y \frac{\partial B_z}{\partial x \mu_m} - \eta_x \frac{\partial B_x}{\partial y \mu_m} \right] \\ (\pi_4 + \pi_5) \frac{1}{R_e \sigma} \left[\eta_x \frac{\partial B_y}{\partial x \mu_m} + \eta_z \frac{\partial B_z}{\partial z \mu_m} - \eta_x \frac{\partial B_z}{\partial y \mu_m} - \eta_z \frac{\partial B_y}{\partial x \mu_m} \right] \\ (\pi_4 + \pi_5) \frac{1}{R_e \sigma} \left[\eta_x \frac{\partial B_z}{\partial x \mu_m} + \eta_y \frac{\partial B_x}{\partial y \mu_m} - \eta_x \frac{\partial B_x}{\partial z \mu_m} - \eta_y \frac{\partial B_z}{\partial x \mu_m} \right] \end{pmatrix},$$

and

$$H'_v = \frac{1}{J} \begin{pmatrix} 0 \\ \frac{1}{R_e} \zeta_{\alpha_i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i1} + (\pi_2 + \pi_3) \sigma_{i1}^{LES}] \\ \frac{1}{R_e} \zeta_{\alpha_i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i2} + (\pi_2 + \pi_3) \sigma_{i2}^{LES}] \\ \frac{1}{R_e} \zeta_{\alpha_i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{i3} + (\pi_2 + \pi_3) \sigma_{i3}^{LES}] \\ \frac{1}{R_e} \zeta_{\alpha_i} u_j [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) \tau_{ij} + (\pi_2 + \pi_3) \sigma_{ij}^{LES}] \\ + \frac{1}{(\gamma-1) Fr M^2 R_e} \zeta_{\alpha_i} [(\pi_1 + \pi_2 + \pi_3 + \pi_4 + \pi_5) q_i + (\pi_2 + \pi_3) Q_i^{LES}] \\ + (\pi_4 + \pi_5) \frac{1}{\mu_m R_{\sigma}} \left[\zeta_{\alpha_i} \frac{\partial}{\partial \omega} \left(\frac{1}{2} \frac{B^2}{\mu_m} \right) - \zeta_{\alpha_i} \left(\frac{\partial B_x}{\partial \omega \mu_m} + \frac{\partial B_y}{\partial \omega \mu_m} + \frac{\partial B_z}{\partial \omega \mu_m} \right) \right] \\ \pi_3 \frac{1}{R_e} \zeta_{\alpha_i} [(\Phi_{ij} + \chi_{ij}^{LES})] \\ (\pi_4 + \pi_5) \frac{1}{R_{\sigma}} \left[\zeta_y \frac{\partial B_x}{\partial y \mu_m} + \zeta_x \frac{\partial B_x}{\partial x \mu_m} - \zeta_y \frac{\partial B_y}{\partial \omega \mu_m} - \zeta_x \frac{\partial B_z}{\partial \omega \mu_m} \right] \\ (\pi_4 + \pi_5) \frac{1}{R_{\sigma}} \left[\zeta_{\omega} \frac{\partial B_y}{\partial \omega \mu_m} + \zeta_z \frac{\partial B_y}{\partial z \mu_m} - \zeta_{\omega} \frac{\partial B_x}{\partial y \mu_m} - \zeta_z \frac{\partial B_x}{\partial y \mu_m} \right] \\ (\pi_4 + \pi_5) \frac{1}{R_{\sigma}} \left[\zeta_{\omega} \frac{\partial B_z}{\partial \omega \mu_m} + \zeta_y \frac{\partial B_z}{\partial y \mu_m} - \zeta_{\omega} \frac{\partial B_x}{\partial z \mu_m} - \zeta_y \frac{\partial B_y}{\partial z \mu_m} \right] \end{pmatrix}.$$

The proposed software suite involves the development of a systematic way of 1) computing derivatives, 2) carrying out TDMA, pentadiagonal solution (PDMA), or Jacobi/Gauss-Seidel iterations, and 3) updating the residuals. The schematic shown below represents the initial concept for the multidisciplinary software, while Appendix A shows a detailed design. The following remarks are in order. Note that within the “engine,” each application (CEM, MHD, FSI, CAA, etc.) could have, as an alternative to the “ π ” formulations above, a separate routine that accesses the same derivative calculation function. The Phase I project focused on the “ π ” formulation. An alternative, optimized approach will be explored in Phase II in order to obtain the most efficient code. This is intended for the applications that have less number of variables than the 8 in the base code. The graphics user interface (GUI) provides the appropriate software branches, as is the case in the current version of the commercial code INSTED. We will also have core and application-specific results and visualization (post-processing).

Programming in Phase I was based on FORTRAN 90, C, and C++. The preliminary compute engine used FORTRAN, whereas C and C++ were used mostly for the interface codes.

IV: Graphical User Interface (GUI)

Although not promised for Phase I, we implemented a preliminary graphics user interface (GUI), to demonstrate the feasibility of a user-friendly interface for the proposed multidisciplinary software. This capability is an absolute necessity for commercialization of the final product. The GUI contains most aspects of the proposed software, except the engine (solver). That is, the left-hand side of the schematic shown below. Sample screens applicable to one of the applications are shown in Appendix B.

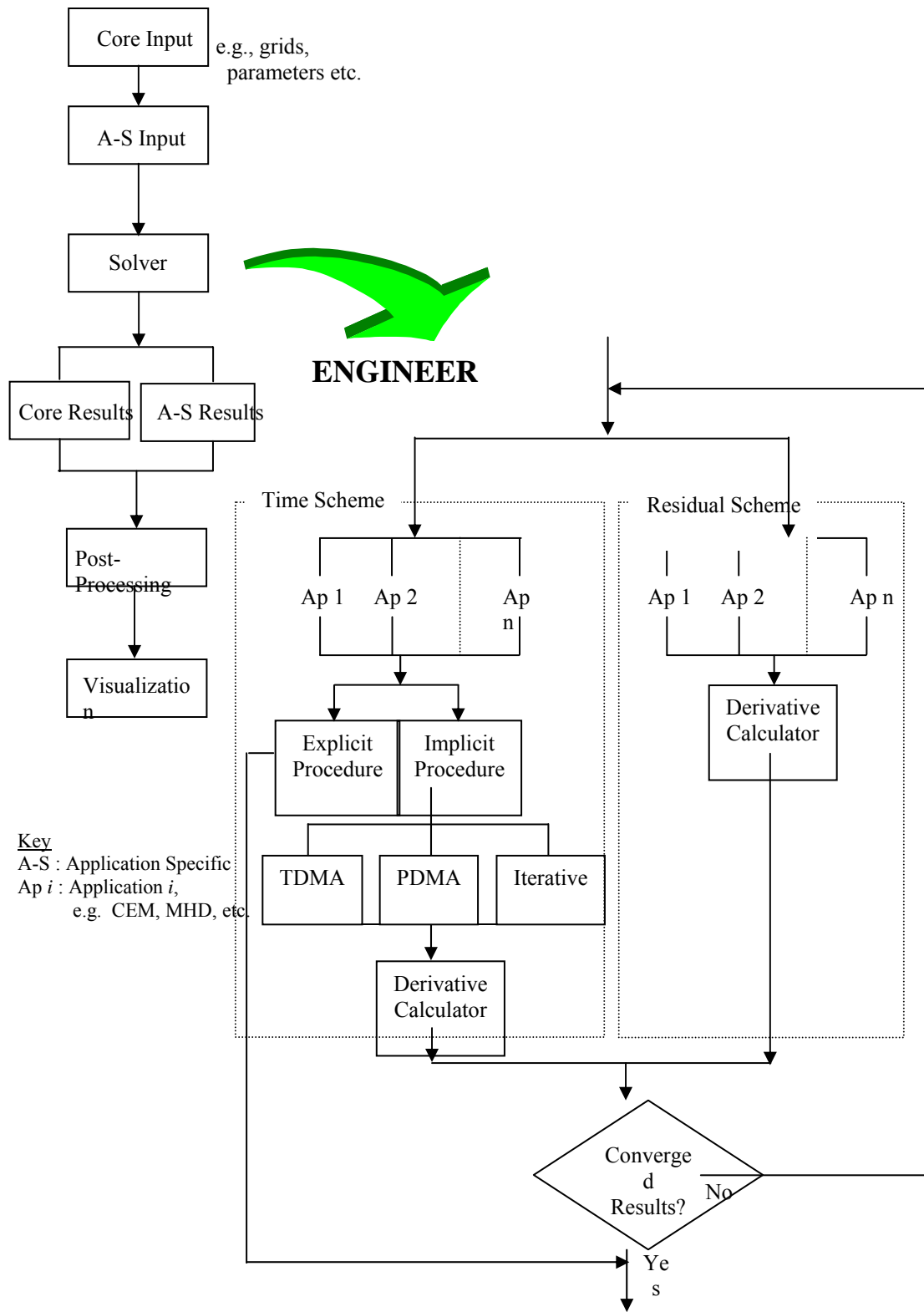


Figure 1 Preliminary Multidisciplinary Software Concept

V. Design of the multidisciplinary Software Suite

A detailed design of the multidisciplinary software is shown in Appendix A.

VI. Demonstration of the multidisciplinary Software Suite

The feasibility of the proposed multidisciplinary software suite was established in Phase I, by ascertaining accuracy and computational efficiency when the proposed design in Appendix A is implemented. The base code for the development of the multidisciplinary code is the Air Force code FDL3D/MGD, which has a default number of variables of 8. We have modified this code to execute in a multidisciplinary environment and have used two problems for evaluation:

- a) MGD (Alfvén wave with ohmic damping). Here, we compare the computational efficiency and accuracy of the original FDL3D/MGD code with those of the preliminary multidisciplinary code derived from it. The CPU times are shown in Table I and the accuracy below in figures 2 through 4. From the table we see that the efficiency of the multidisciplinary code is comparable to that of the original MGD code for both the Runge-Kutta and Beam-Warming time integration methods. Note that the CPU times shown are for 100 time steps and the Beam-Warming calculations use 3 sub-iterations per time step. This exercise shows that the multidisciplinary software suite is quite feasible, in relation to the base code.
- b) Acoustic scattering by a concept X24C vehicle. This problem is interesting for a couple of reasons: it represents a complex geometry and involves only 5 variables (as opposed to the 8 in the base code for the multidisciplinary software). Therefore, the associated overhead is expected to challenge the multidisciplinary code relative to a dedicated code for acoustic scattering. (See Ladeinde et al., 2001.) The initial results confirm our suspicion (not shown). However, a preliminary optimization technique was found to show great promise for the multidisciplinary software suite when the number of variables is much fewer than that in the base code. The latter will be fully developed in Phase II.

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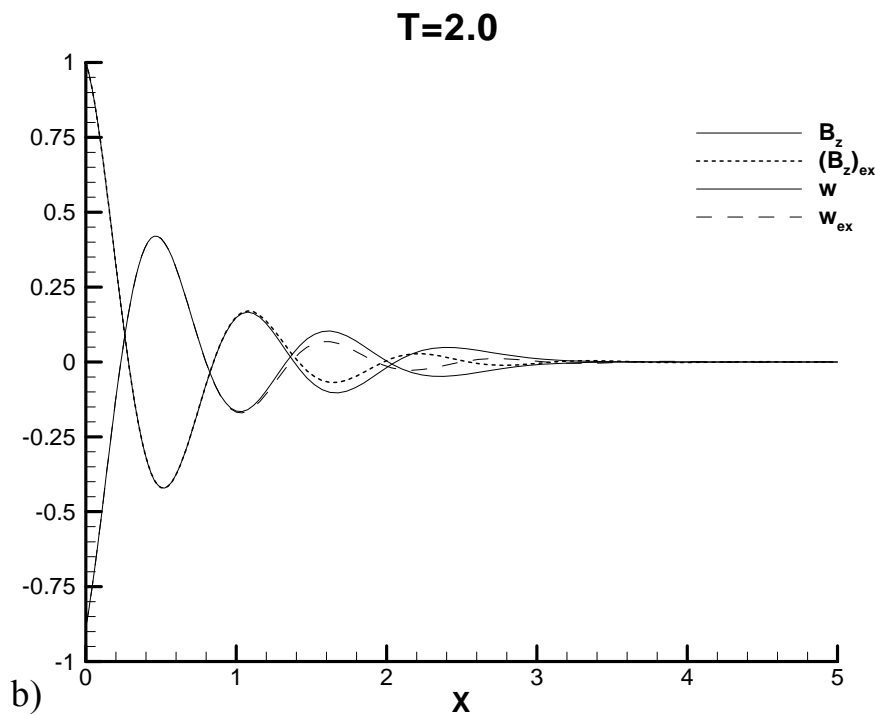
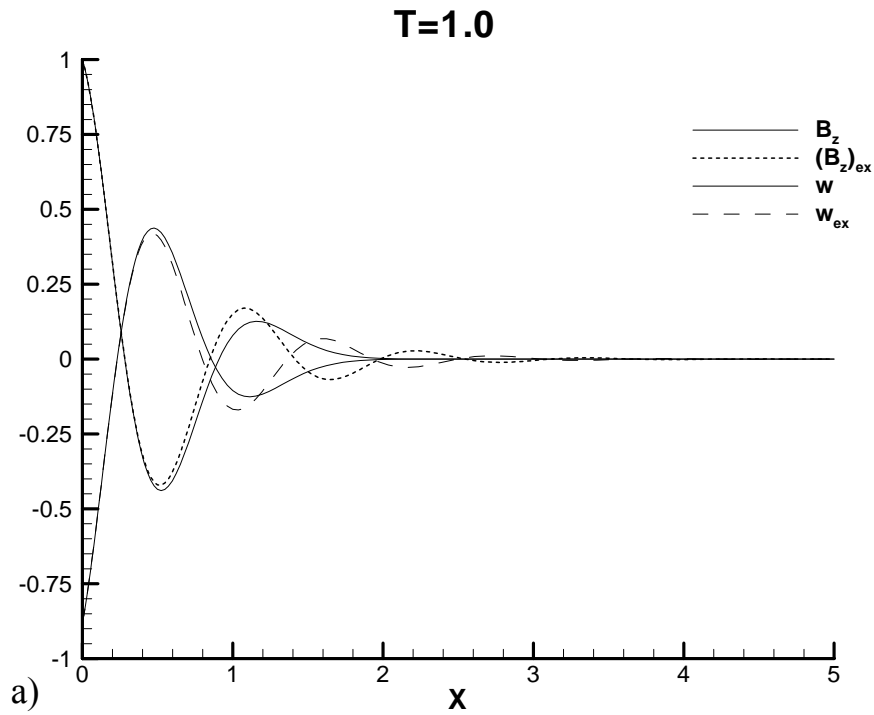


Fig.2 Results from Multi-disciplinary code using Runge-Kutta Scheme

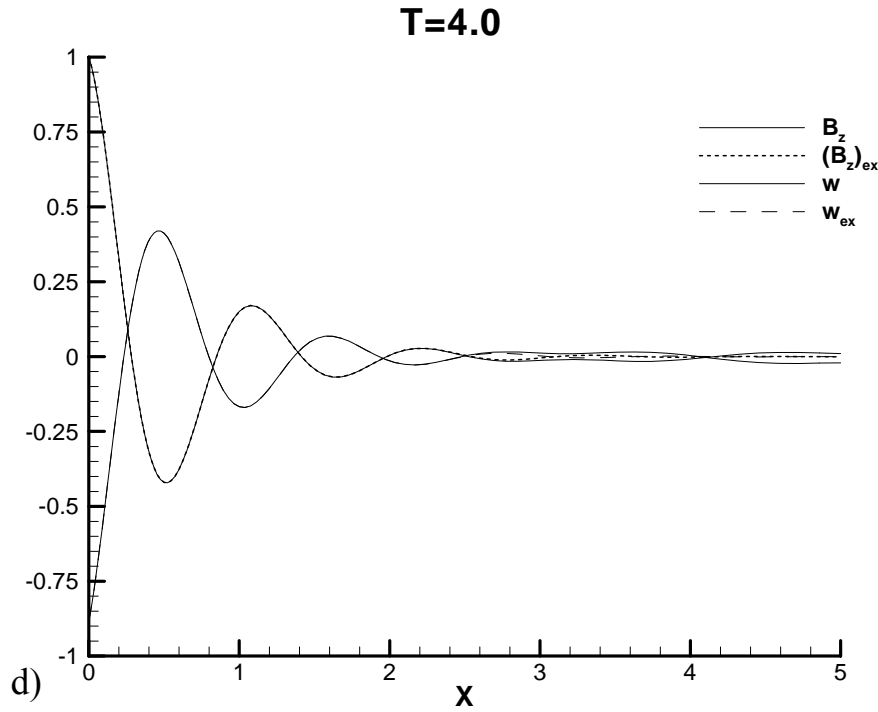
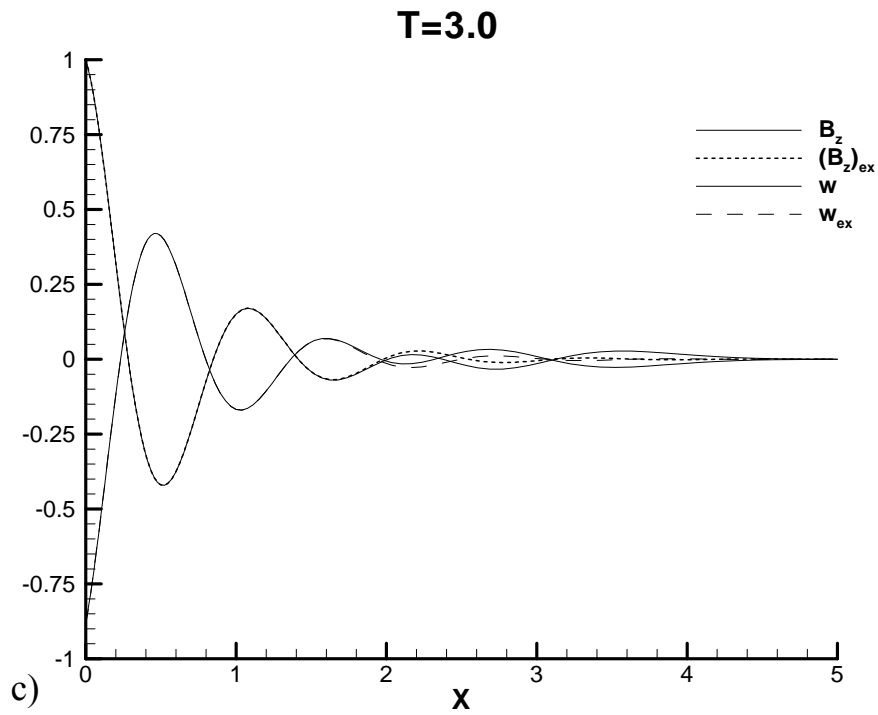


Fig.2 Results from Multi-disciplinary code using Runge-Kutta scheme

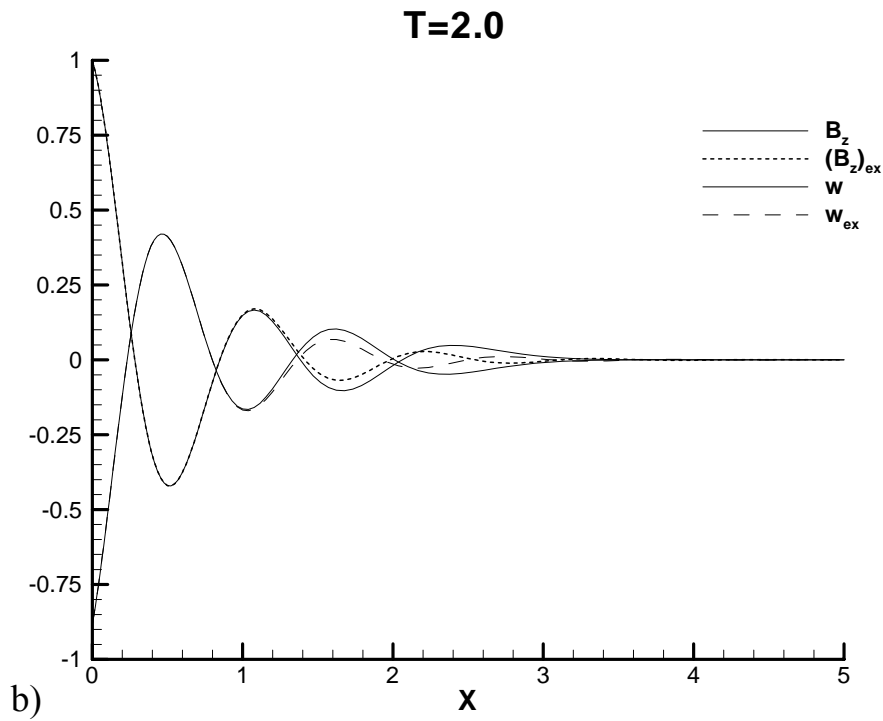
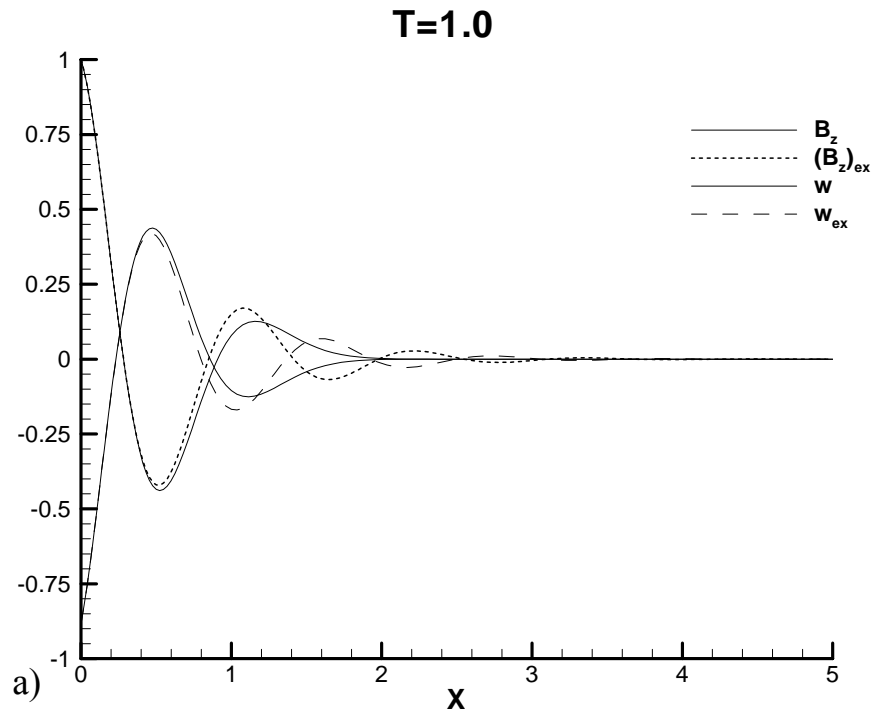


Fig.3 Results from Multi-disciplinary code using Runge-Kutta scheme
 (Reduced Mesh System: 101x3x3)

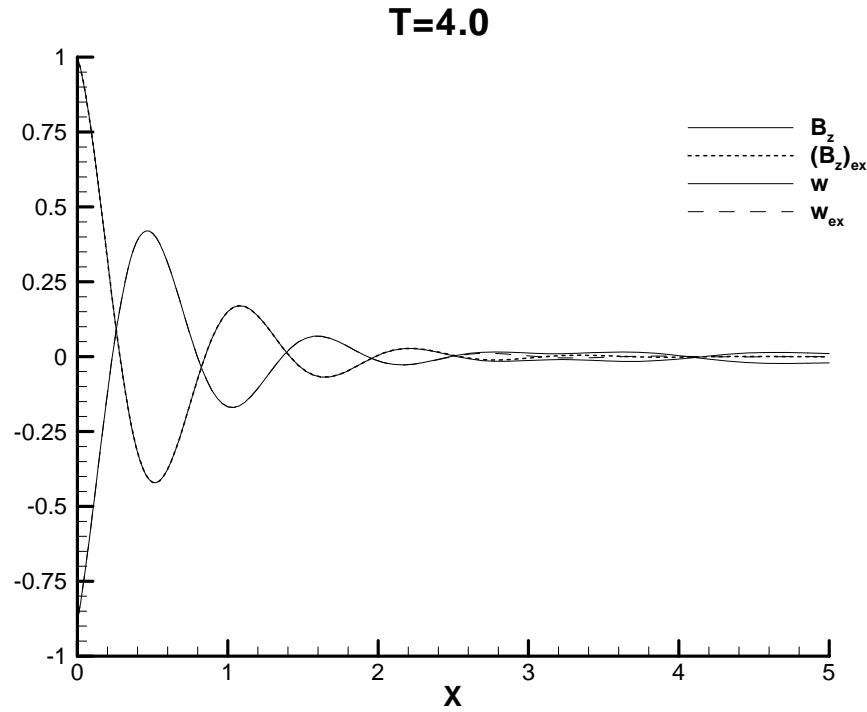
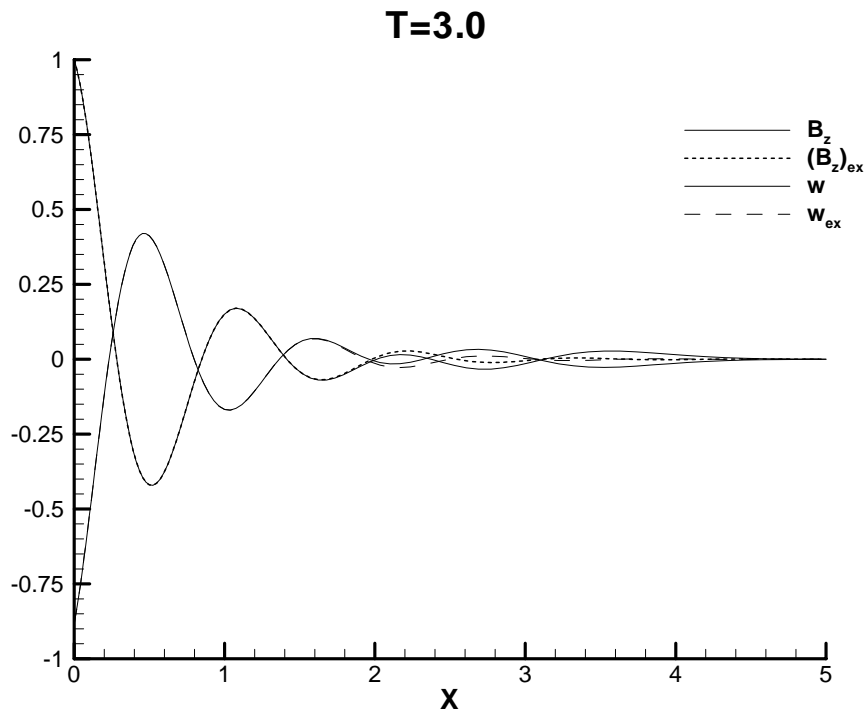


Fig.3 Results from Multi-disciplinary code using Runge-Kutta scheme
 (Reduced Mesh System: 101x3x3)

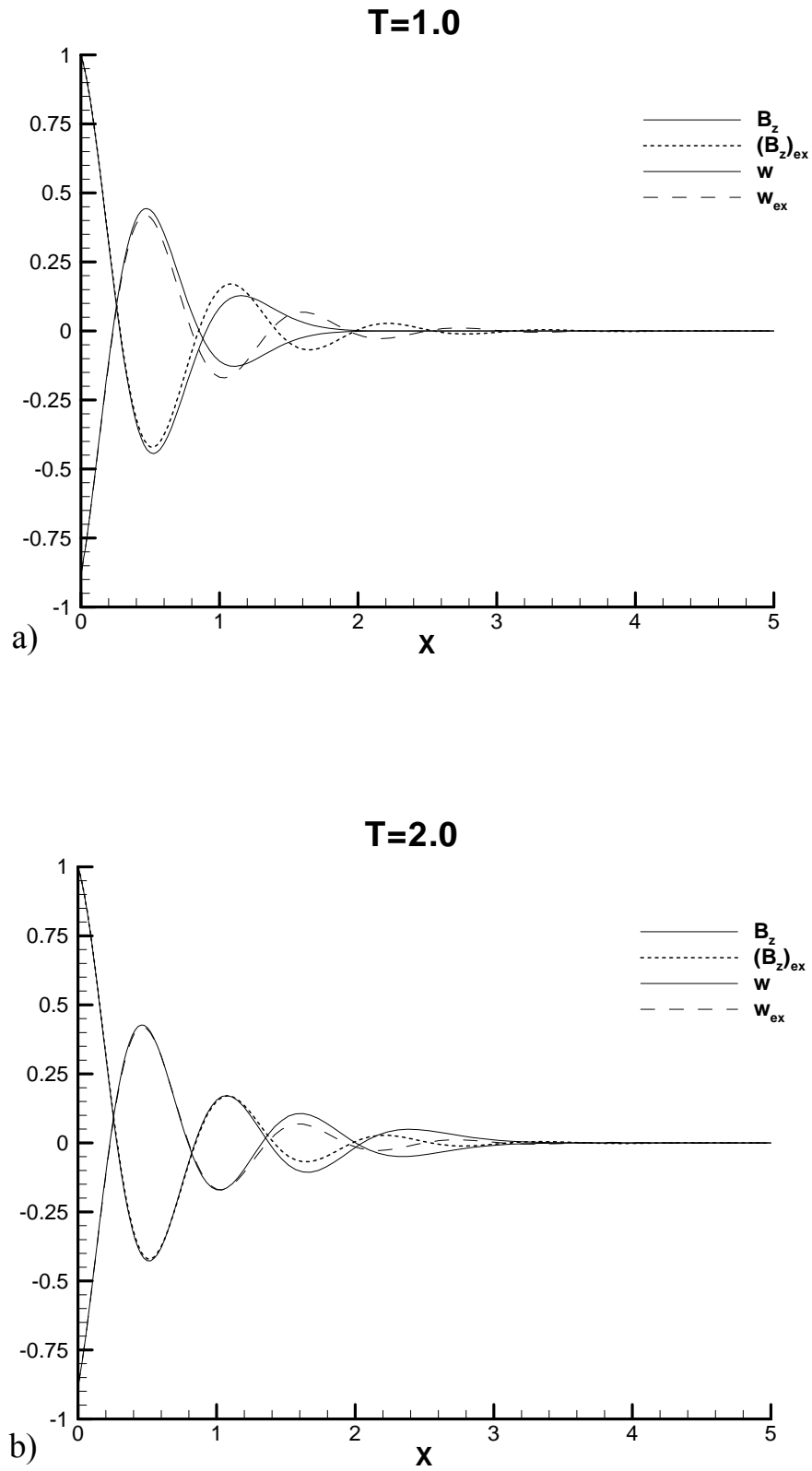


Fig.4 Results from Multi-Disciplinary code with Beam-Warming scheme

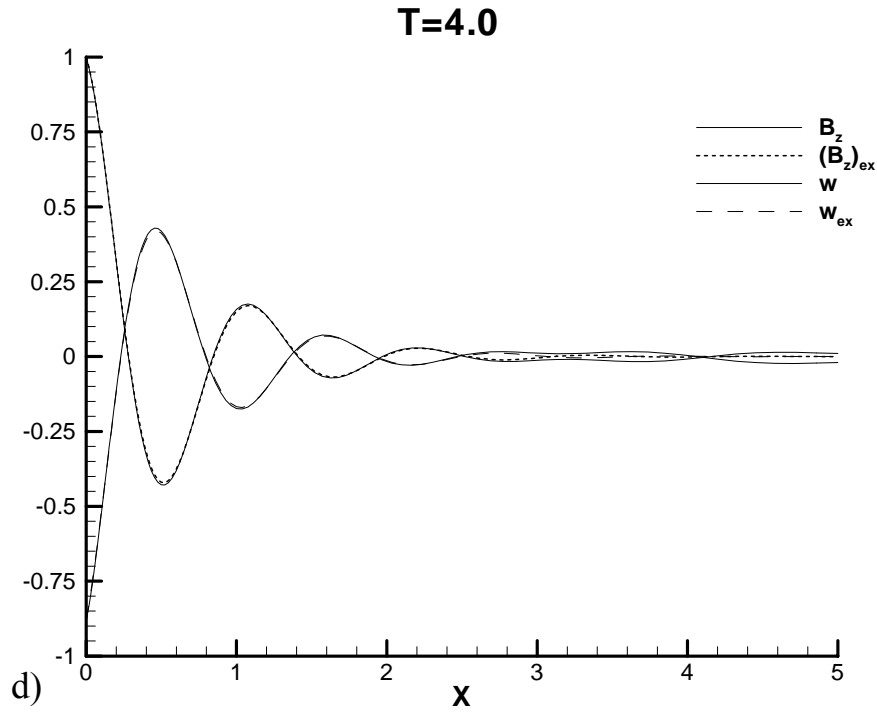
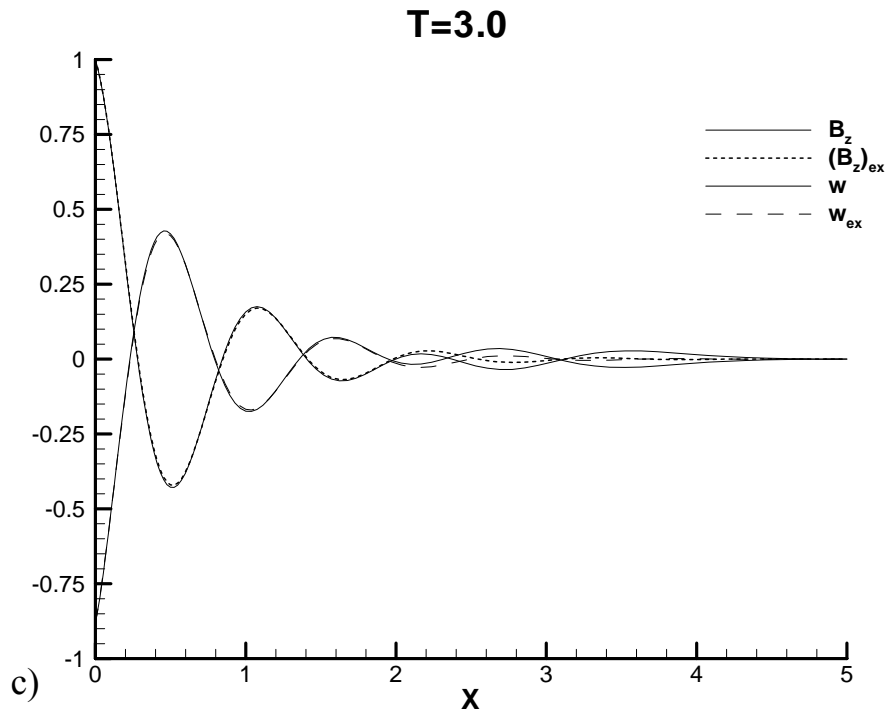


Fig.4 Results from Multi-Disciplinary code with Beam-Warming scheme

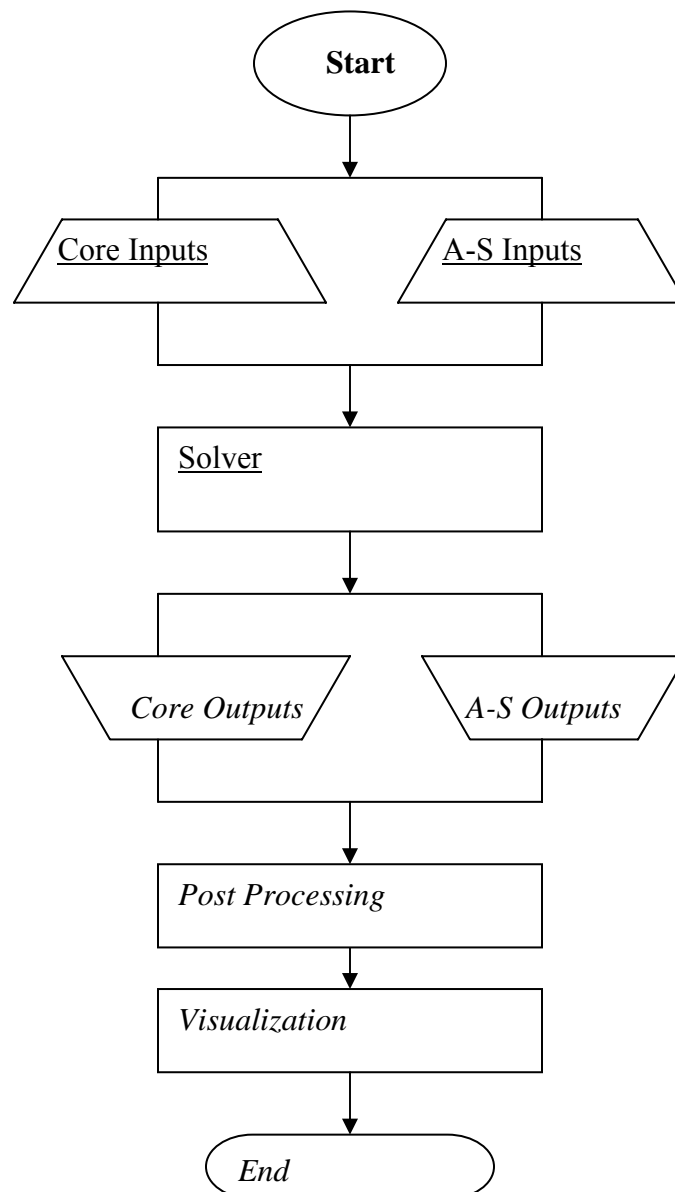
APPENDIX A

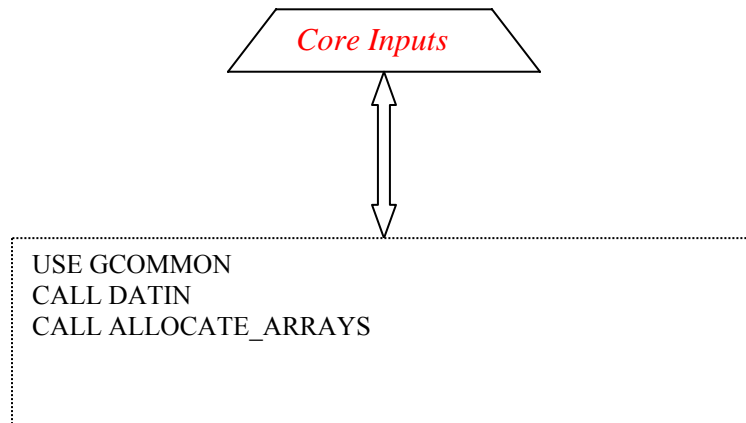
Design of the Multi-disciplinary Software Suite

● New Control-Variable Table

	DNS/NS	LES/NS	Combustion	CAA	DNS/MHD	LES/MHD	CEM
Π1	1						
Π2		1					
Π3			1				
Π4				1			
Π5					1		
Π6						1	
Π7							1

● Flow-Chart





1. In “Gcommon.f90” add code segment:

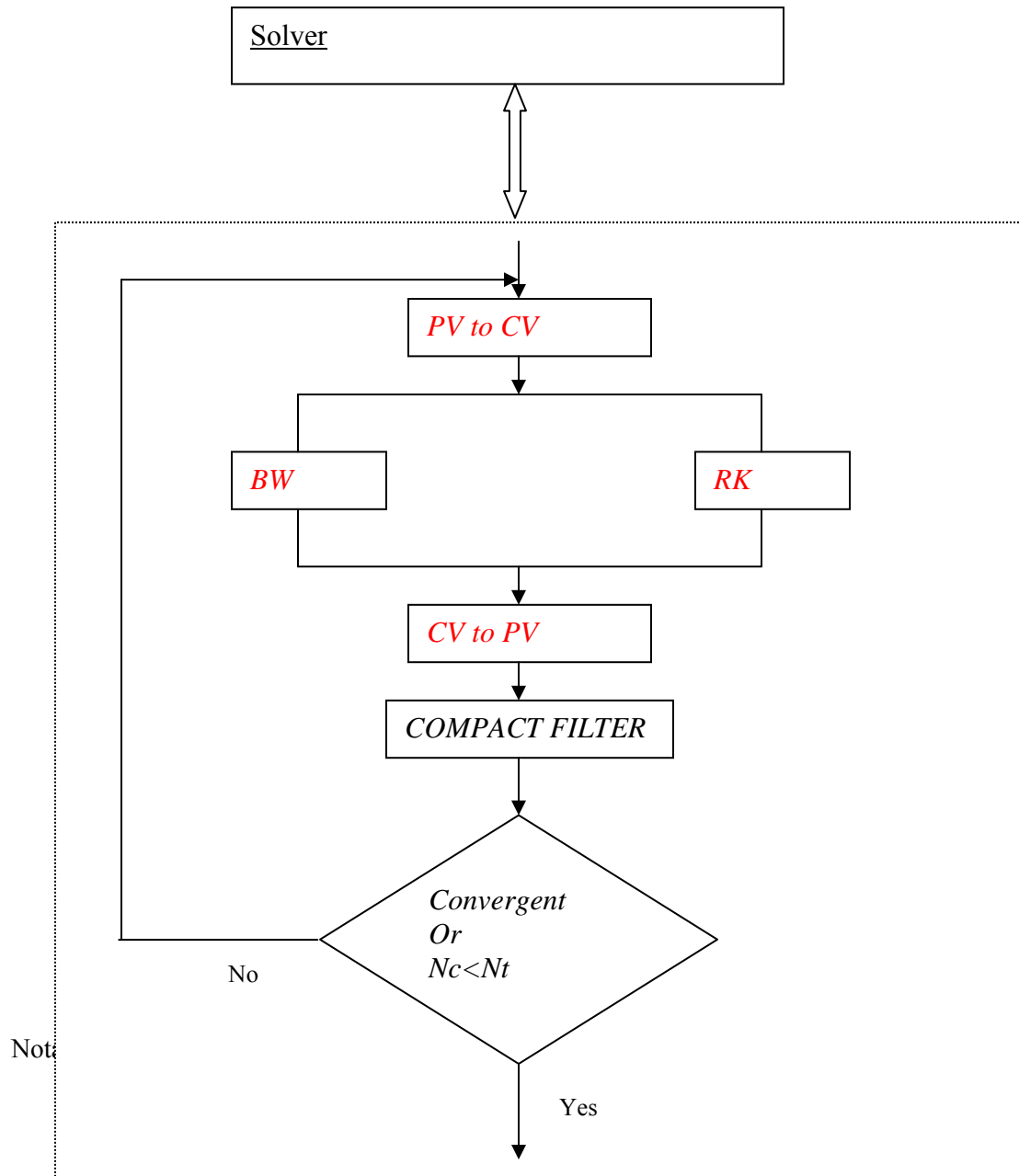
2. In “I

```

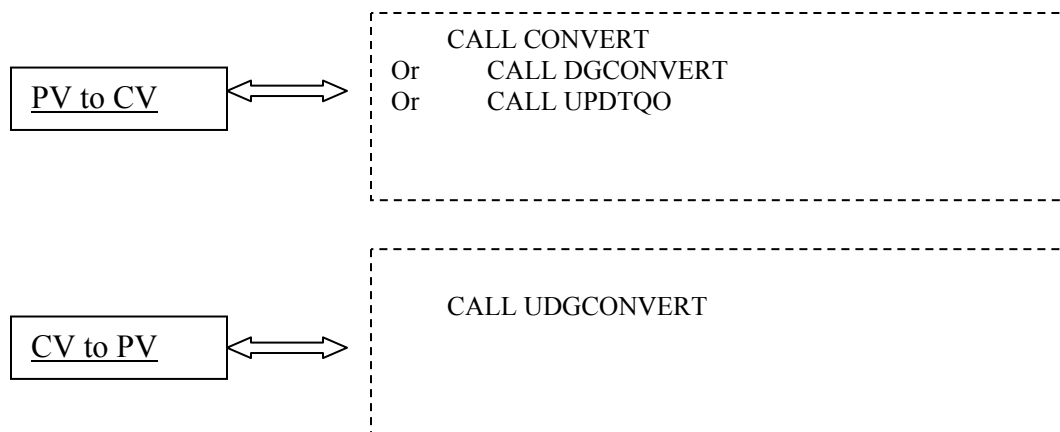
MULTI_TYPE=0
READ *, MULTI_DSCP
MULTI_DSCP=MULTI_DSCP/10
MULTI_TYPE (MULTI_DSCP)=1
WRITE *, "WARNING SIGNS"

```

- **Modification on Highlighted Blocks**



● **Modifications on Transformation between Primitives and Conservatives**



COMMON CONTROL LOGICS:

```

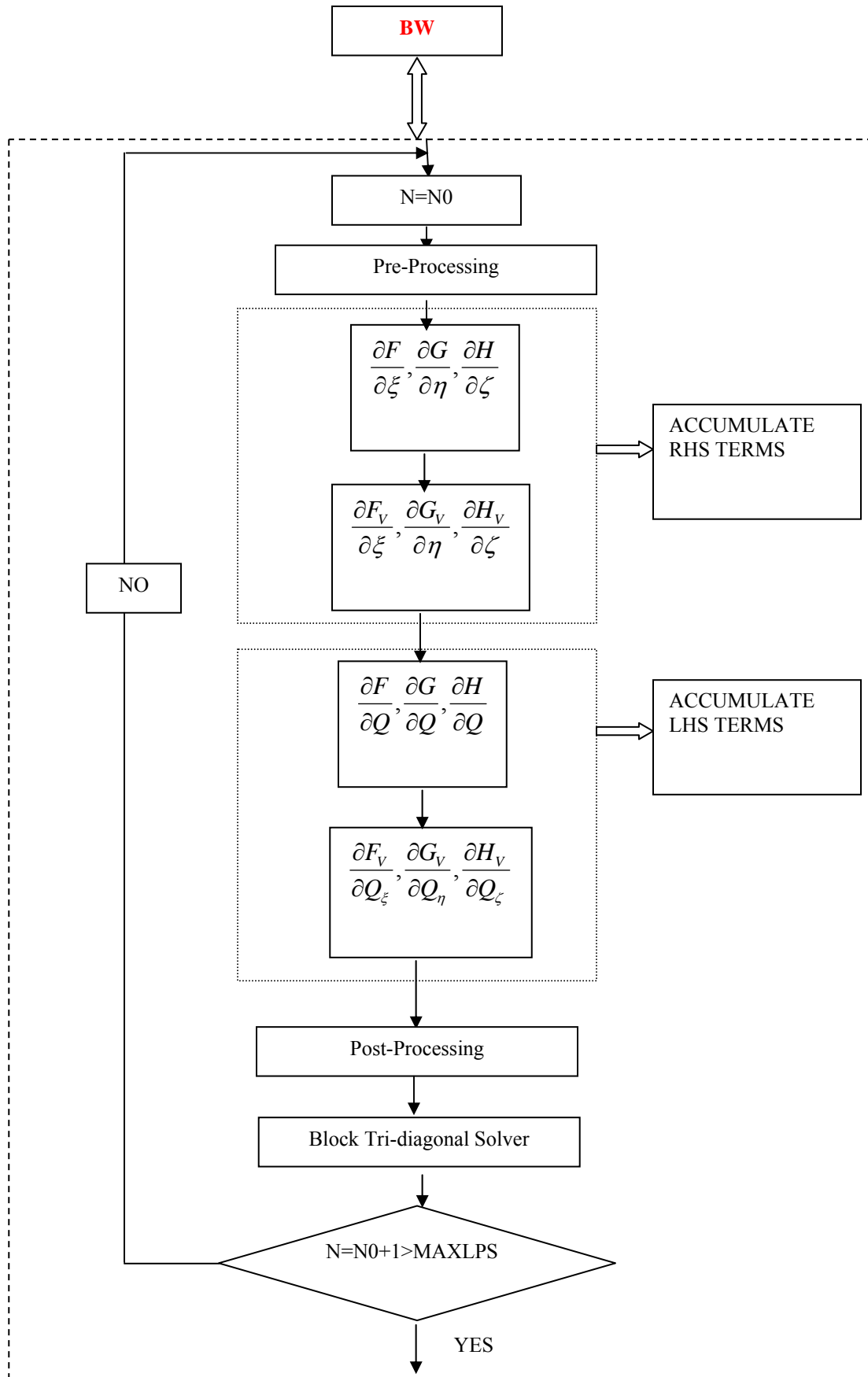
    VARIABLE_ARRAY=0                ! INITIALIZATION
                                     !
                                     ! CASE-SELECT STRUCTURE
                                     !
    MULITI_ONE: SELECT CASE (MULTI_DSCP)
                CASE (1:6)
                    VARIABLE_ARRAY=BASIC TERMS in NS
                CASE (7)
                    VARIABLE_ARRAY=CEM TERMS
    END SELECT MULITI_ONE

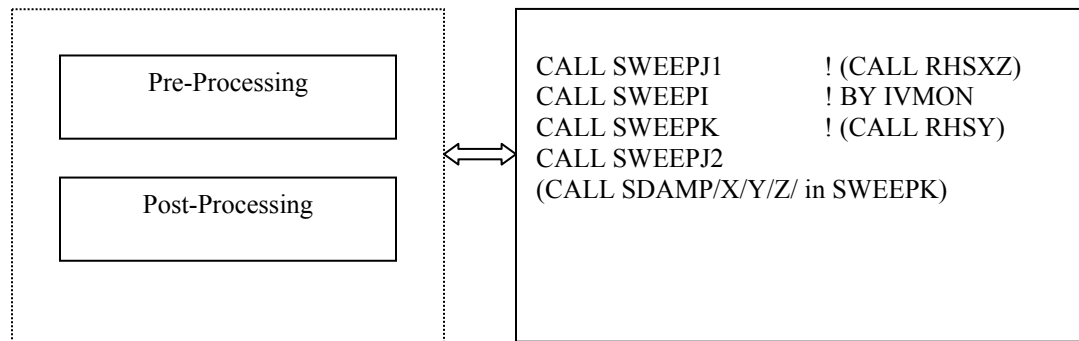
    MULITI_TWO: SELECT CASE (MULTI_DSCP)
                CASE (3)
                    VARIABLE_ARRAY=REACTING SPECIES
                CASE (4:5)
                    VARIABLE_ARRAY=B FIELDS
    END SELECT MULITI_TWO
  
```

Notes:

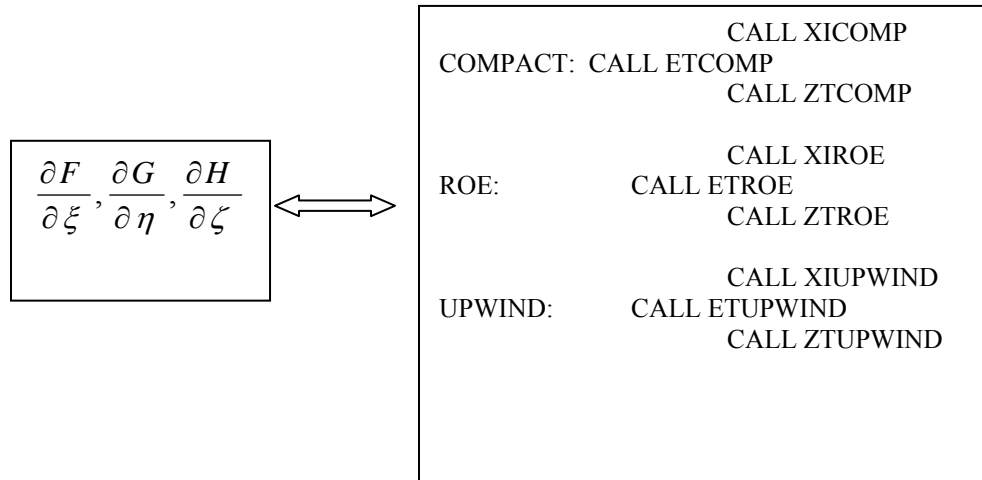
1. Replace the VARIABLE_ARRAY by different WORK ARRAYS in different subroutines, namely,
 - a) TEMP () in CONVERT.F90;
 - b) RHS () in DGCONVERT.F90
 - c) QOLD () in UPDTQO.F90

● **Modifications on Beam-Warming Solver**

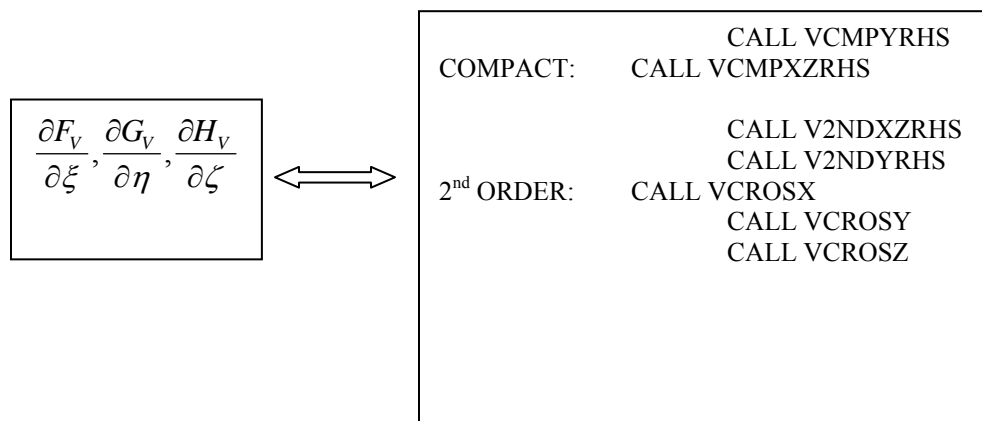




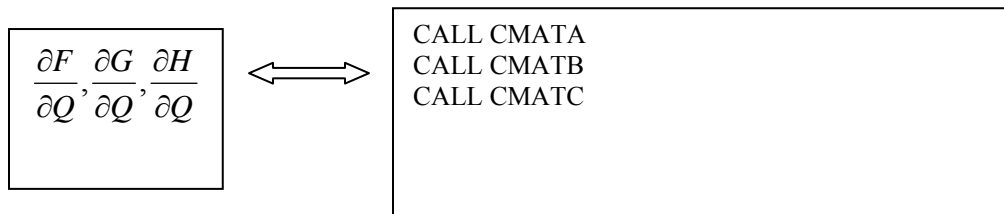
2.



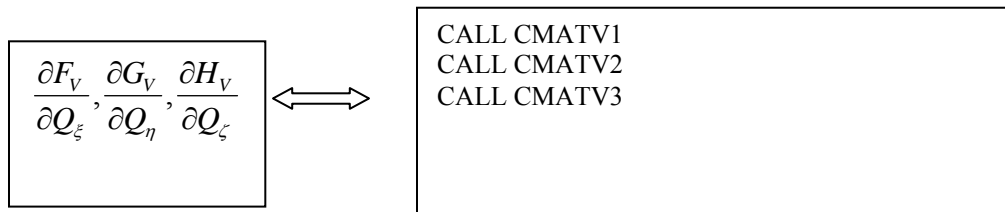
3.



4.



5.



6. The same CASE-SELECT logics as used above are applied here. The work arrays specifically are:

- a) WRK (*,*,*,1), TEMP (*,*,*) and RHS (*,*,*) in SWEEP/I/J1/J2/K/.F90
- b) WRK (*,*,*,1) in /XI/ET/ZI/COMP.F90
- c) WRK (*,*,*,1) and RHS (*,*,*) in VCMP/XZ/Y/RHS.F90 and VCROS/X/Y/Z/.F90
- d) ALCL (*,*,*) in CMAT/A/B/C/.F90 and CMAT/V1/V2/V3/.F90
- e) WRK (*,*,*,*) in SDAMP/X/Y/Z/.F90

7. Note: Roe, Upwind, 2nd-Order differencing schemes are currently not implemented for the multi-disciplinary computation.

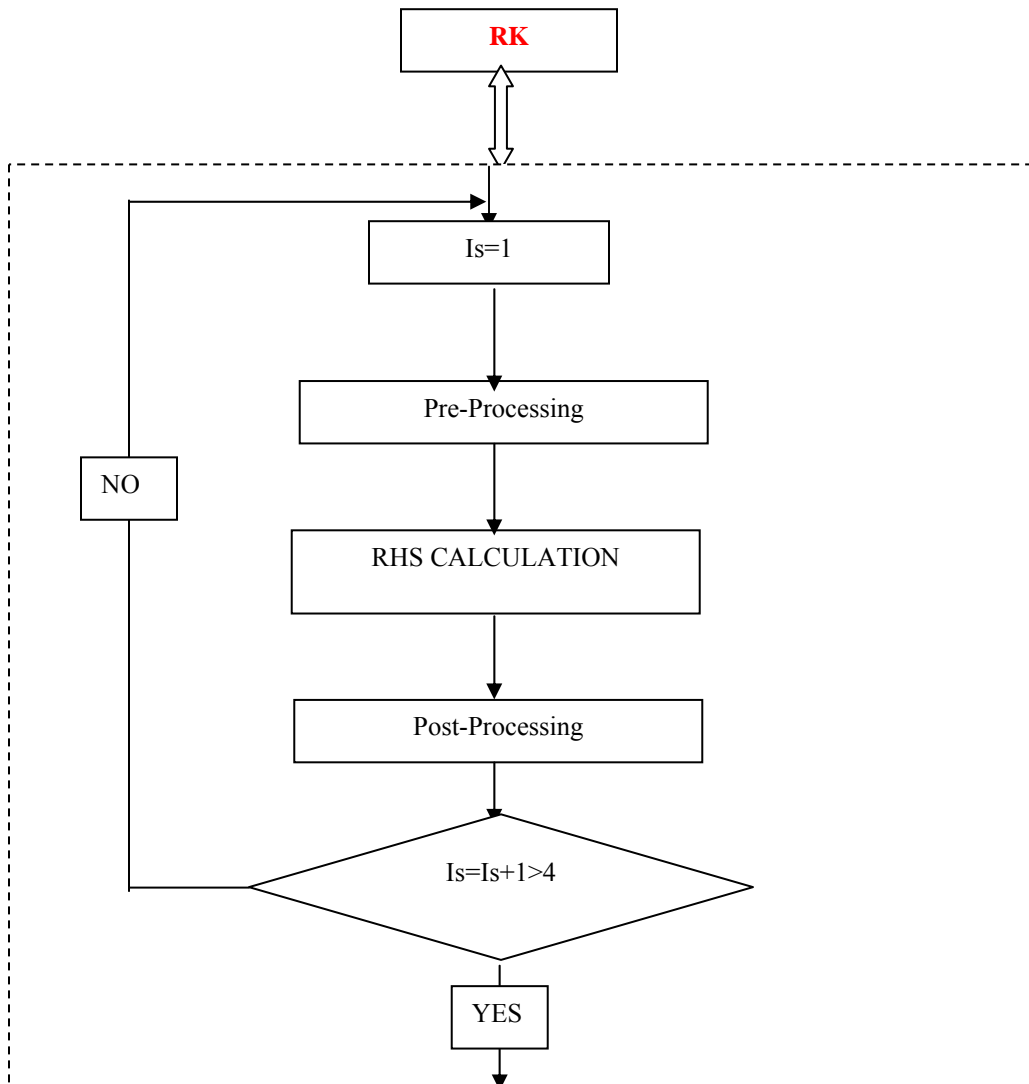
8. ADD SUBROUTINE MULTI_SOURCE.F90 for Beam-Warming procedure. The algorithm is:

LHS of BW (0)

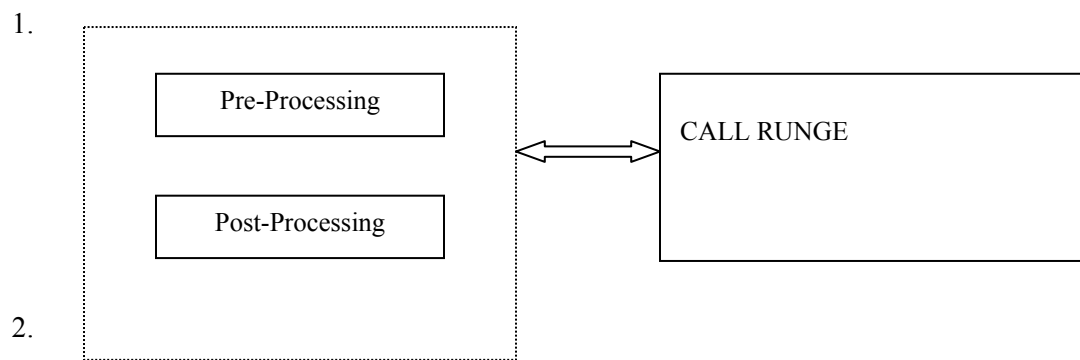
$$= \text{RHS of BW (0)} + \frac{\Delta t}{1 + \Phi} S$$

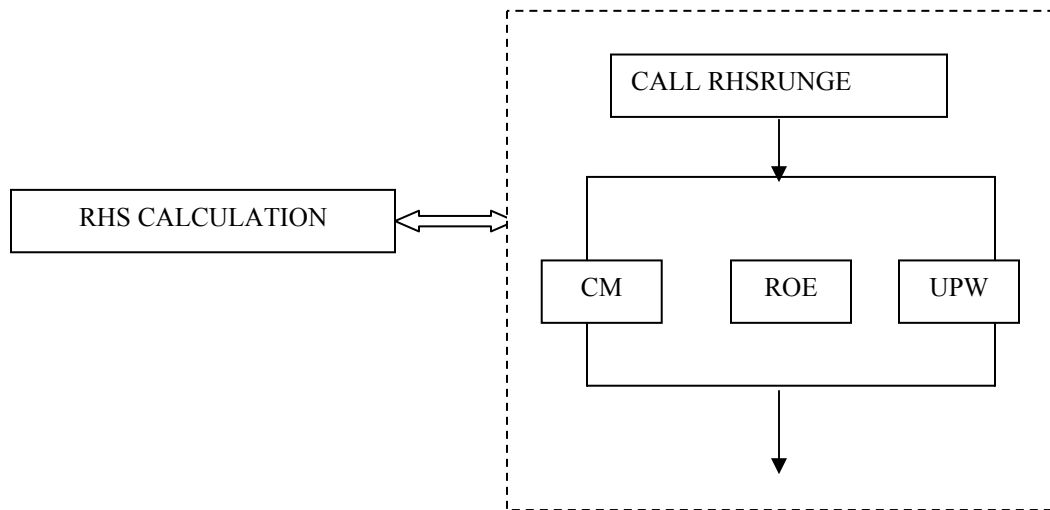
Where BW (0) represents the original Beam-Warming procedure and the expression of the source term S is described in my notebook.

● Modifications on Runge-Kutta Solver



Detail Descriptions of the implementation:





3. The same CASE-SELECT logics as used above are applied here. The work arrays, specifically, are:

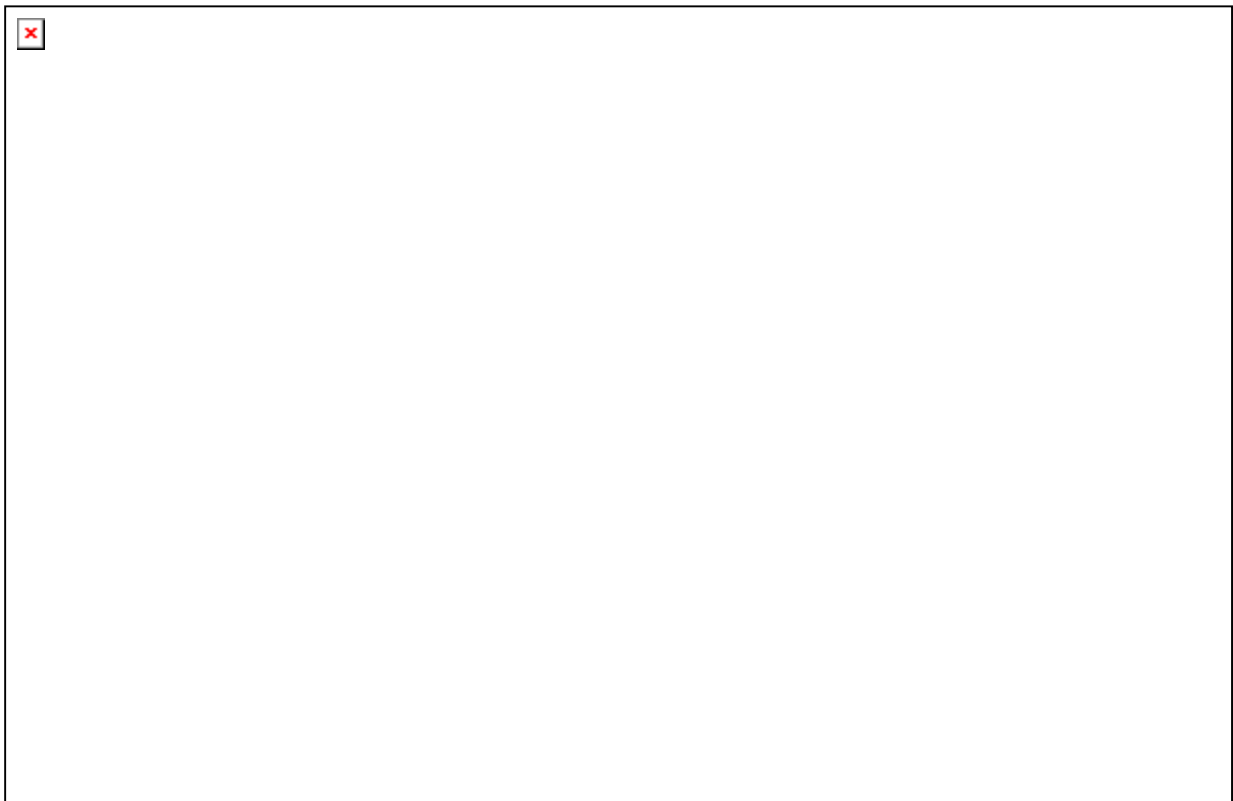
- a) TEMP (*,*,*) and QOLD (*,*,*,*) in RUNGE.F90
- b) WRK (*,*,*,1) in /XI/ET/ZT/COMP.F90
- c) WRK (*,*,*,1) and RHS (*,*,*) in VCMP/XZ/Y/RHS.F90 and VCROS/X/Y/Z/.F90

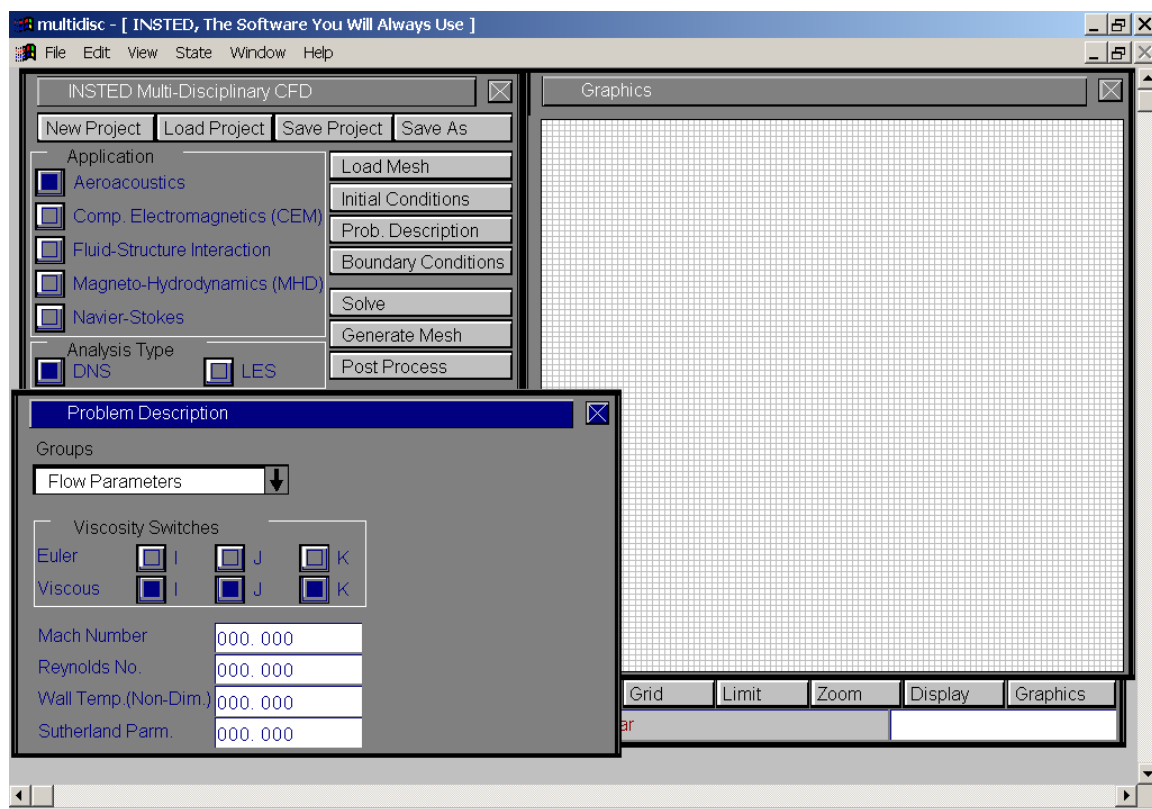
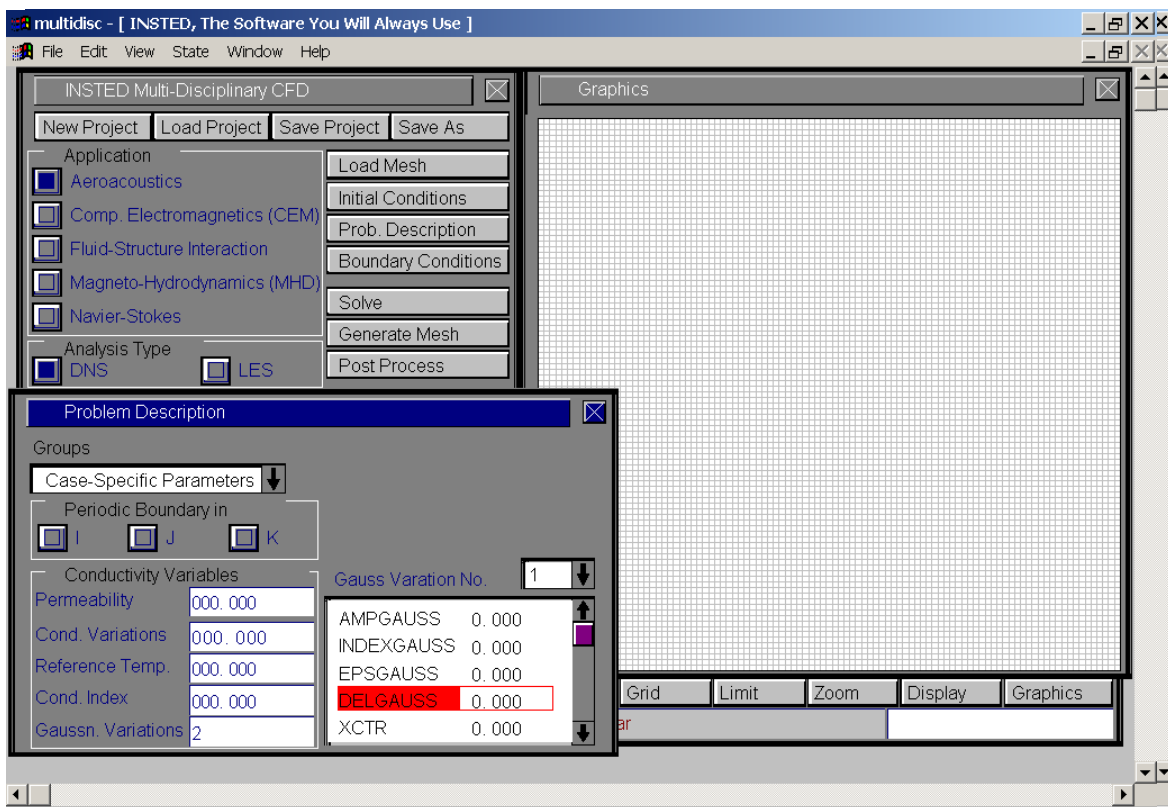
4. ADD SUBROUTINE MULTI_SOURCE.F90 for Runge-Kutta procedure. The algorithm is:

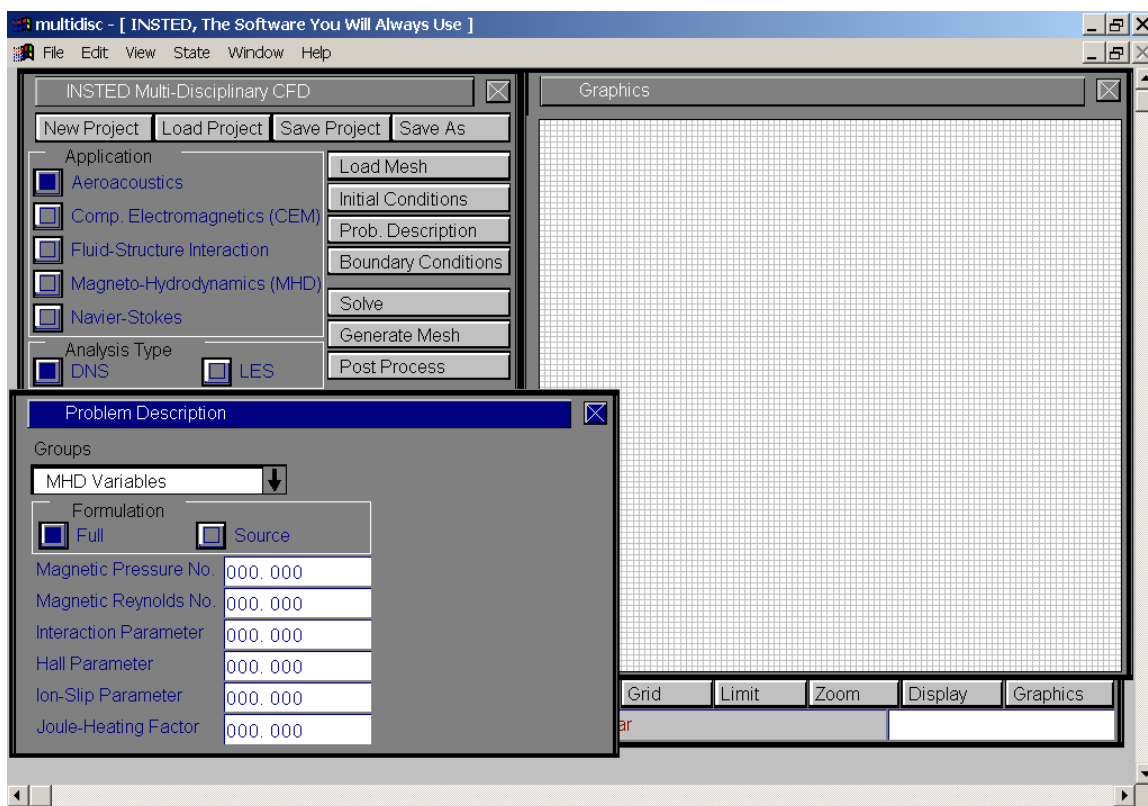
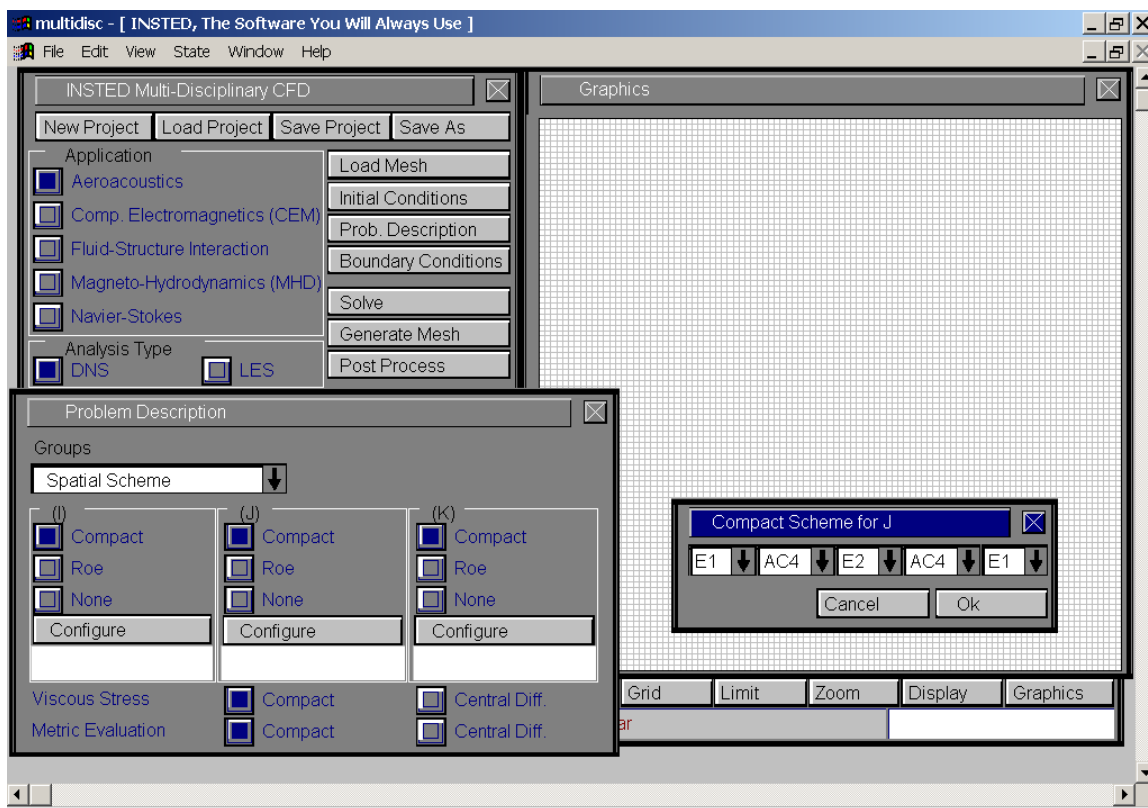
$$\text{LHS of RK (0)} \\ = \text{RHS of RK (0)} + \Delta t \cdot J \cdot S$$

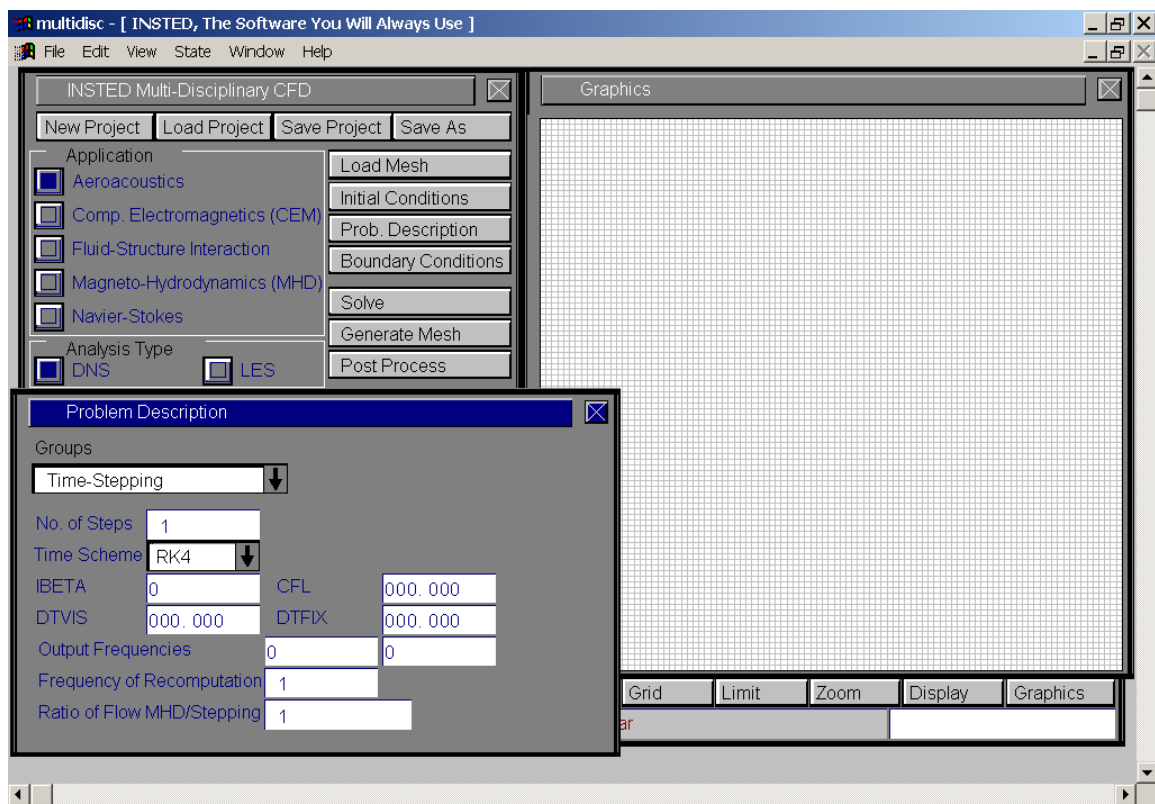
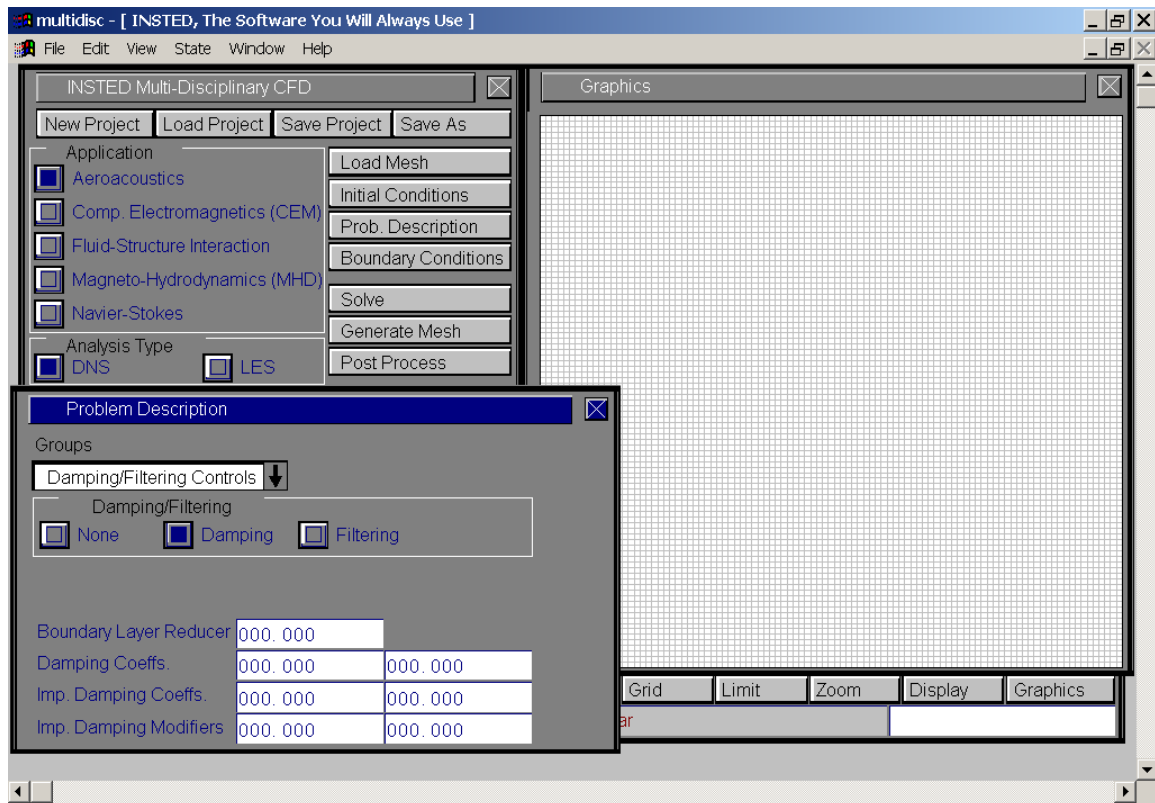
Where RK (0) represents the original Runge-Kutta procedure and the expression of the source term S is described in my notebook.

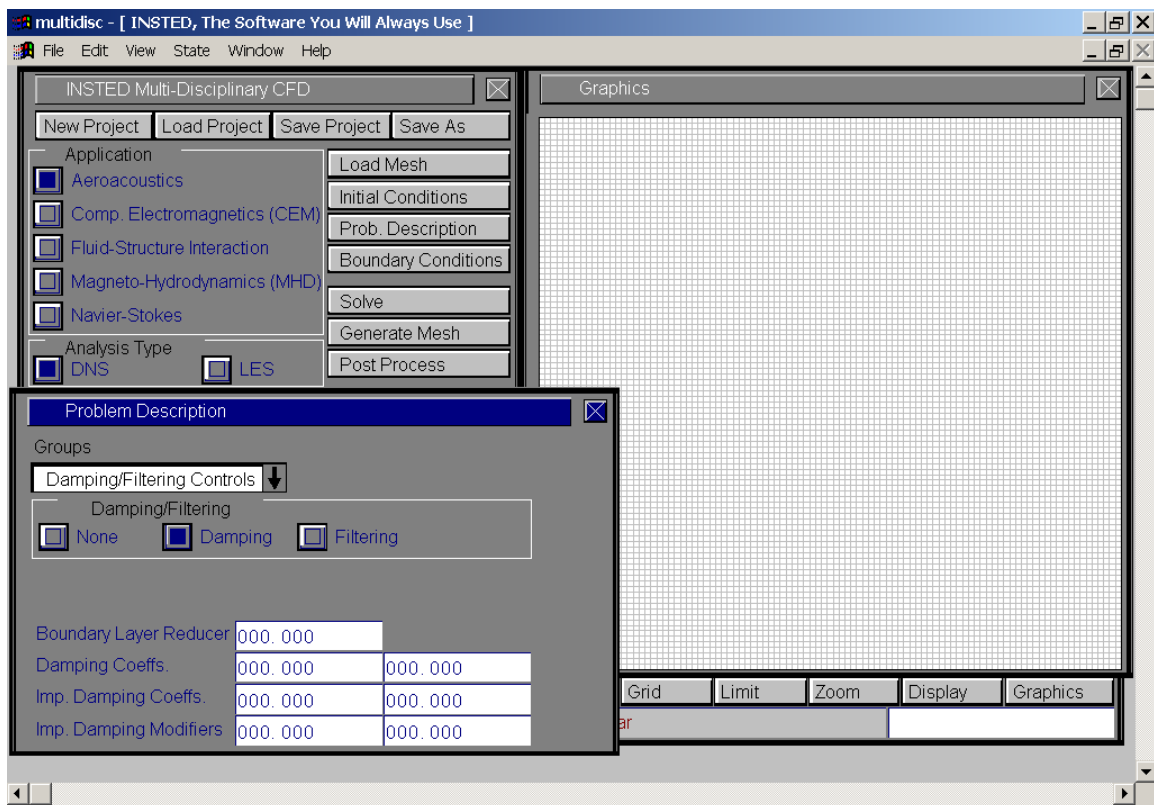
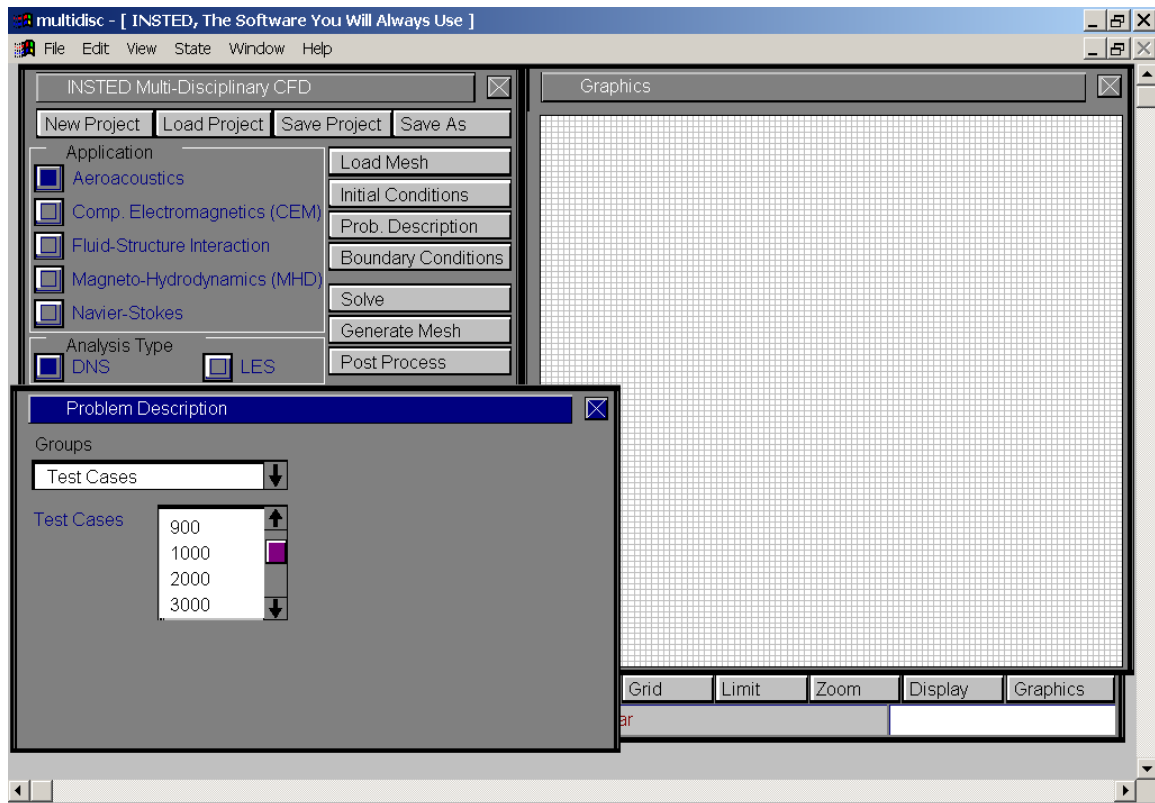
Appendix B: Sample GUI Screens

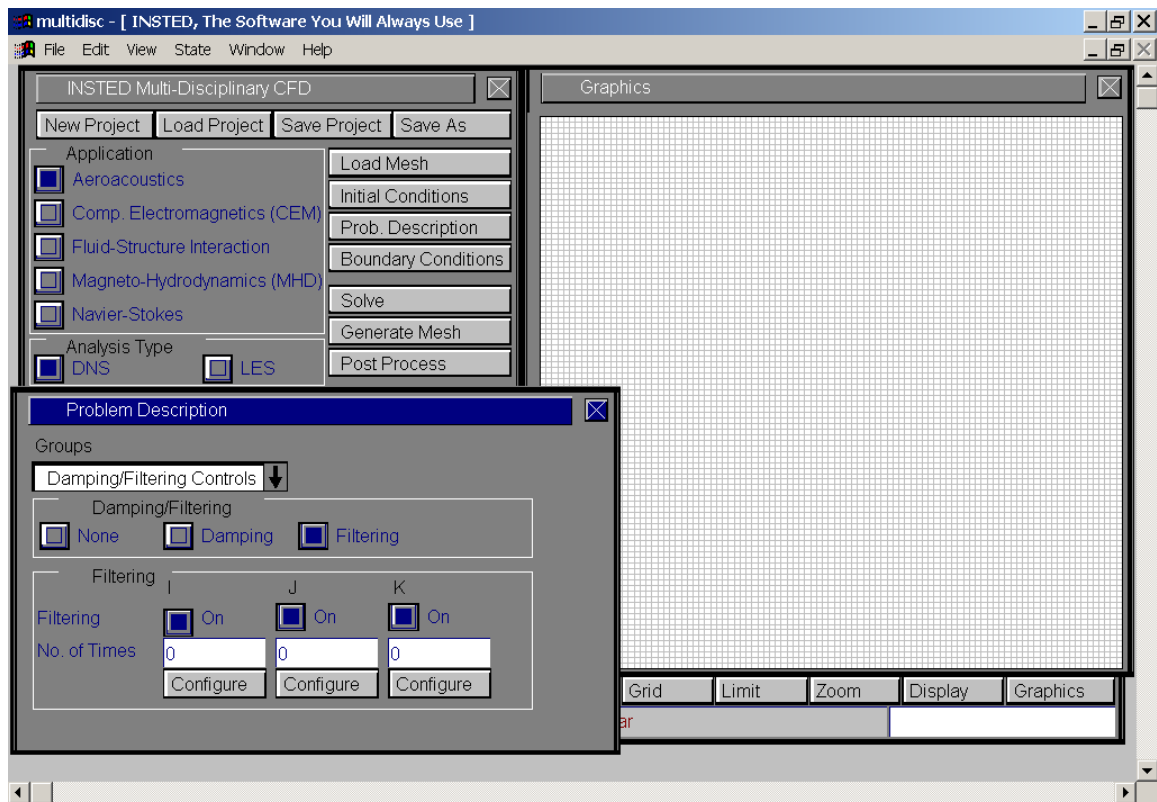
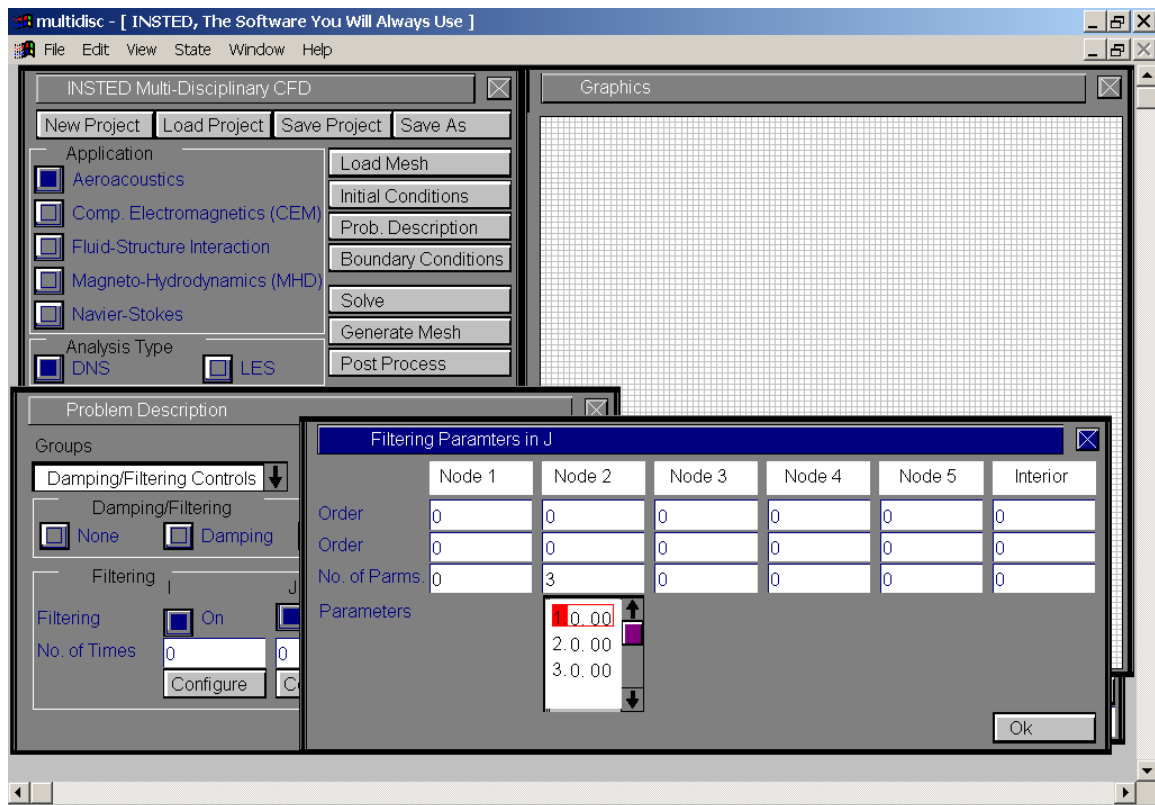












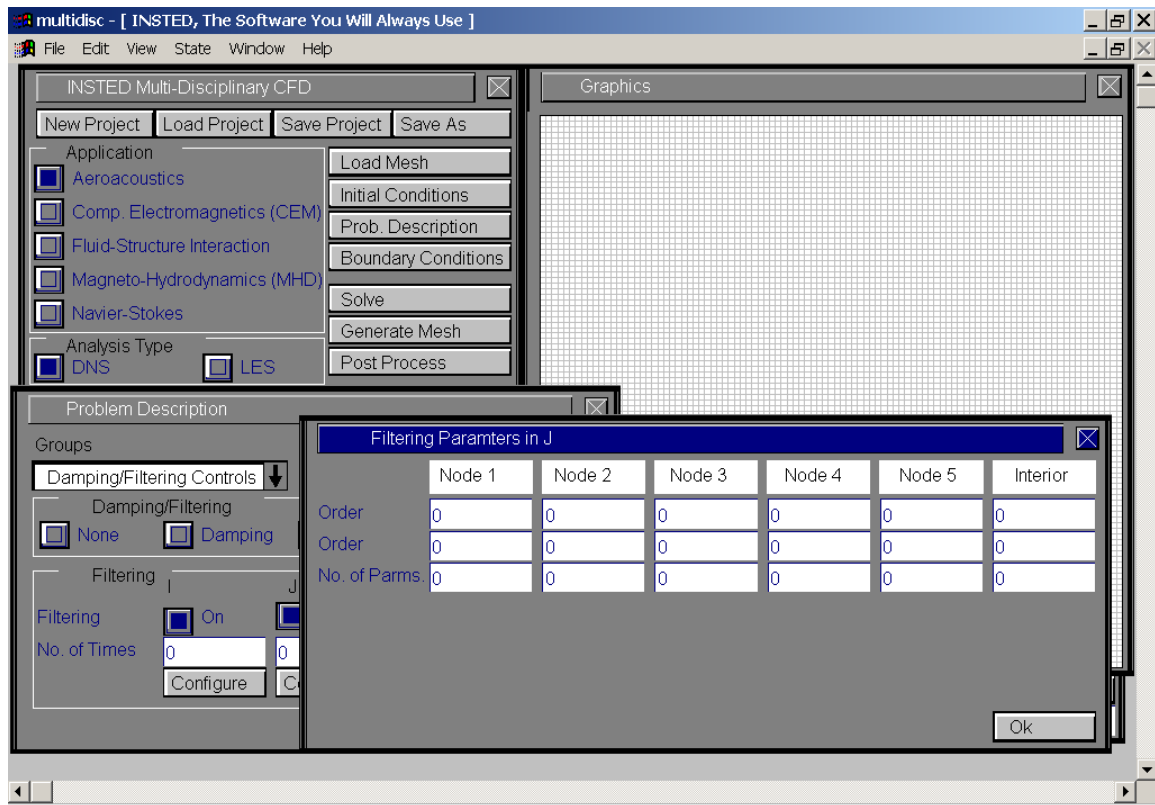


Table I: Comparison of CPU time (seconds) for the calculation of Alfvén wave with ohmic damping. The CPU times are reported for 100 time steps. The Beam-Warming scheme uses 3 sub-iterations per time step.

Code Type	Grid Size	CPU time (seconds)	
		Runge-Kutta	Beam-Warming
Base code	101×11×11	3035.9	4742.1
Multidisciplinary code	101×11×11	2990.9	4787.0
Multidisciplinary code	101×3×3	3632.0	95.09

Appendix C: List of FDL3D Files Modified

The following is a list of FDL3d/MGD project files that were modified in the preliminary conversion of the code to a multidisciplinary suite. Note that some files contain multiple routines/procedures.

bndry.f90, cmata.f90, cmatb.f90, cmatc.f90, cmatv1.f90, cmatv2.f90, cmatv3.f90, convrt.f90, datin.f90, deriv.f90, dgconvrt.f90, etcomp.f90, fdl3d_ice.f90, fdtry.f90, gcomon1.f90, met2nd.f90, multi_src.f90, nirhs.f90, output.f90, pirhs.f90, rhsrunge.f90, runge.f90, sdampx.f90, sdampy.f90, sdampz.f90, sdampz1.f90, sdiagx.f90, sdiagy.f90, sdiagz.f90, sweepi.f90, sweepj1.f90, sweepj2.f90, sweepk.f90, tmstep.f90, txiirhs.f90, tzetrhs.f90, udgconvrt.f90, updtqo.f90, vcmpxrhs.f90, vcmpyrhs.f90, writetec.f90, wrtfield.f90, wrthist.f90, xicomp.f90, ztcomp.f90

APPENDIX D: Grid for Second Test Problem for the Multidisciplinary Software

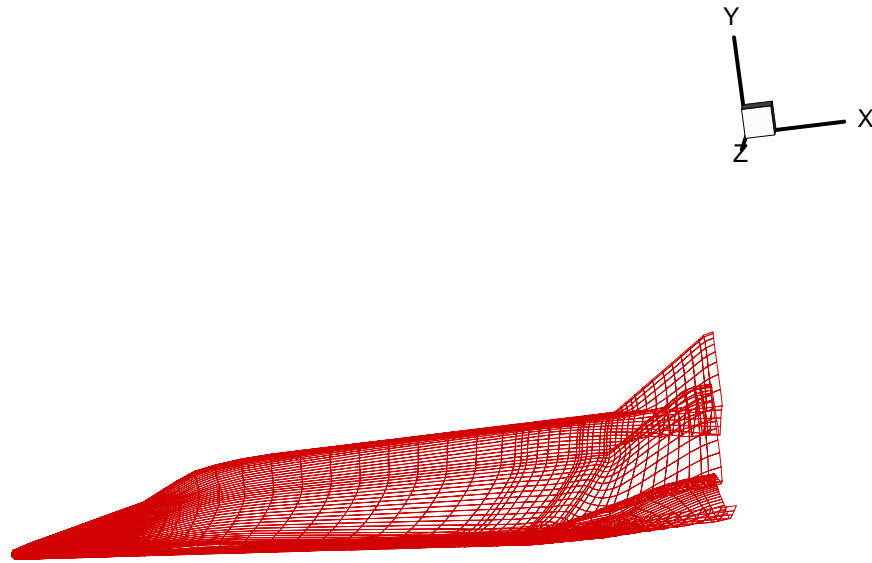


Fig.5 Coarse grid model of X24C Reentry Vehicle showing the surface mesh.